



JUNE 2-6

2024

**ANAHEIM**  
CALIFORNIA

# POSTERS

Updated May 2 with NEW Poster Code Numbers.

This document includes a detailed listing for all poster sessions, Monday – Thursday.

A final program (PDF) will be created over the coming weeks and will combine this document with a schedule overview, orals, workshops, and an author index.

Conference attendees are encouraged to use the digital conference program tools, Planner & App, available here:

<https://www.asms.org/conferences/annual-conference/online-planner-app>

## POSTER OVERVIEW

### MONDAY POSTERS

Set up all Monday posters  
6:30 - 9:00 am

**Odd-numbered posters present**  
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

**Even-numbered posters present**  
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Monday posters  
5:00 - 8:00 pm

Ambient Ionization: Applications .....	001-020
Antidoping, Cannabis, and Opioid Detection .....	021-031
Carbohydrates .....	032-040
Data-Independent Acquisition .....	041-073
Drug Discovery / DMPK / ADME .....	074-098
Drug and Metabolite Analysis .....	099-125
Education: Teaching MS .....	126-130
Elemental Analysis .....	131-135
Energy: Petroleum, Biofuels, and Algae .....	136-155
Environmental: General .....	156-192
Environmental: Pharmaceuticals and Pesticides .....	193-206
Extractables & Leachables .....	207-217
Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements .....	218-236
Fundamentals: Ion Activation/Dissociation .....	237-247
Fundamentals: Ion Structure/Energetics/Reactions .....	248-263
Fundamentals: Molecular Modeling/Quantum Mechanical Calculations .....	264-269
Glycomics .....	270-295
H/D Exchange: Hardware, Software and Methodology .....	296-307
H/D Exchange: Protein Structure/Function .....	308-338
Imaging MS: Pharmaceuticals, Metabolites, Lipids, and Glycans I .....	339-363
Imaging: Spatially-Resolved Omics I .....	364-383
Industry: Trace Analysis, Quality Control, and Automation .....	384-393
Informatics: Metabolomics and Lipidomics .....	394-425
Informatics: Peptide ID and Quantification .....	426-456
Ion Mobility: Applications I .....	457-476
Lipids: ID and Structural Analysis I .....	477-496
Lipids: Profile Analysis .....	497-523
Metabolomics: General .....	524-555
Metabolomics: Untargeted Metabolite Profiling I .....	556-589
Microorganisms and the Microbiome I .....	590-614
Nucleic Acids and Oligonucleotides I .....	615-640
Peptides: Identification and Fragmentation Mechanisms .....	641-646
Peptides: PTM Identification .....	647-673
Process Development MS .....	674-685
Proteins: Complexes/Non-covalent Interactions .....	686-721
Proteomics: New Approaches I .....	722-741
Single Cell MS I .....	742-780
Small Molecules: Qualitative and Quantitative Analysis .....	781-803
Viruses and Virus-Like Particles .....	804-821

### TUESDAY POSTERS

Set up all Tuesday posters  
6:30 - 9:00 am

**Odd-numbered posters present**  
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

**Even-numbered posters present**  
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Tuesday posters  
5:00 - 8:00 pm

Ambient Ionization: Applications II .....	001-021
Biomarkers: Quantitative Analysis I .....	022-047
Disease Biomarkers .....	048-062
Environmental: General II .....	063-098
Exposomics .....	099-117
Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements II .....	118-137
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Fundamentals: Native MS .....	155-171
High Throughput MS I .....	172-196
Imaging MS: Instrumentation .....	197-206
Imaging MS: Pharmaceuticals, Metabolites, Lipids, and Glycans II .....	207-229
Imaging: Spatially-Resolved Omics II .....	230-248
Informatics: Algorithms and Statistical Advances .....	249-283
Instrumentation: General .....	284-299
Ion Mobility: Applications II .....	300-319
Isotope Labeling and Fluxomics Applications .....	320-325
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Lipids: General .....	347-378
Lipids: ID and Structural Analysis II .....	379-397
Metabolomics: Clinical Applications .....	398-414
Metabolomics: Identification of Unknown Metabolites .....	415-427
Metabolomics: Sample Preparation .....	428-437
Metabolomics: Untargeted Metabolite Profiling II .....	438-471
Microorganisms and the Microbiome II .....	472-496
Nanoscale/Microfluidic and Capillary Electrophoresis Separations and MS .....	497-509
Neuroscience and Neurodegenerative Disease Research I .....	510-530
Nucleic Acids and Oligonucleotides II .....	531-557
Peptidomics and Immuno-peptidomics .....	558-587
Phosphopeptides and Phosphoproteins .....	588-608
Plant Biology and Biotechnology .....	609-620
Protein Therapeutics: Structural Characterization .....	621-650
Proteins: Conformation Analysis and Structural Biology .....	651-673
Proteomics: Chemoproteomics .....	674-706
Proteomics: Clinical Applications I .....	707-729
Proteomics: Infectious Diseases .....	730-734
Proteomics: New Approaches II .....	735-754
Single Cell MS II .....	755-773
Small Molecules: Qualitative and Quantitative Analysis II .....	774-794
Stable Isotope Labeling .....	795-809

## POSTER OVERVIEW

### WEDNESDAY POSTERS

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**Even-numbered posters present**  
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Wednesday posters  
5:00 - 8:00 pm

Ambient Ionization: Fundamentals and Instrumentation.....	001-008
Antibodies & Antibody Drug Conjugates .....	009-039
Artificial Intelligence in MS Instrumentation.....	040-064
Biomarkers: Discovery I .....	065-101
Biomarkers: Quantitative Analysis II.....	102-127
Cancer Research I .....	128-165
Clinical Analysis I.....	166-196
Covalent Labeling and Chemical Crosslinking .....	197-222
Drug Discovery: Qualitative and Quantitative .....	223-247
Environmental: General III .....	248-284
Fundamentals: Unconventional Approaches in MS .....	285-293
Glycoproteins I .....	294-324
High Throughput MS II .....	325-349
Imaging MS: Method Development I.....	350-383
Informatics: Protein ID and Quantification.....	384-396
Informatics: Workflow and Data Management.....	397-430
Instrumentation: Mini/Portable/Fieldable MS.....	431-442
Instrumentation: New Developments in Mass .....	443-458
Ion Mobility: FAIMS/DMS .....	459-465
Ion Mobility: General .....	466-479
LC/MS: Chromatography and Software .....	480-492
LC/MS: Sample Preparation II .....	493-512
Metabolomics: Targeted and Quantitative Analysis.....	513-533
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Proteins: General and Membrane .....	642-657
Proteins: PTMs I .....	658-677
Proteomics: Intact Proteins and Top .....	678-708
Proteomics: Quantitative I .....	709-743
Proteomics: Tissue .....	744-772
Single Cell MS III .....	773-794
Synthetic Polymers .....	795-808
Toxicology .....	809-821

### THURSDAY POSTERS

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6:30 - 9:00 am

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Remove all Thursday posters  
**2:30 - 3:00 pm**

Antibodies & Antibody Drug Conjugates II.....	001-032
Art, Archaeology & Paleontology .....	033-041
Artificial Intelligence in MS Instrumentation and Applications II.....	042-069
Biomarkers: Discovery II .....	070-099
Biomarkers: Quantitative Analysis III .....	100-126
Cancer Research II .....	127-160
Clinical Analysis II .....	161-187
Covalent Labeling and Chemical Crosslinking II.....	188-212
Drug Discovery: Qualitative and Quantitative Analysis II .....	213-237
Epigenetic Modifications.....	238-244
Food Safety: General .....	245-273
Forensics .....	274-303
Fundamentals: Ion Spectroscopy .....	304-308
Fundamentals: Ionic Clusters, Nanomaterials, and Catalysis .....	309-311
Fundamentals: Ionization .....	312-325
GC/MS: Instrumentation and Applications .....	326-364
Glycoproteins II .....	365-393
High Mass Accuracy/High Performance MS: Applications .....	394-412
Imaging MS: Computational Methods, Software, and Analysis.....	413-429
Imaging MS: Disease Markers .....	430-442
Imaging MS: Method Development II .....	443-476
Informatics: General, SRM, and DIA .....	477-484
Informatics: Multiomics Integration .....	485-502
Instrumentation: New Concepts .....	503-519
Instrumentation: New Developments in Ionization and Sampling .....	520-538
Ion Mobility: Fundamentals .....	539-544
Ion Mobility: Structure .....	545-565
LC/MS: General .....	566-594
Lipids: Targeted and Quantitative Analysis.....	595-627
MALDI: Applications .....	628-638
MALDI: Innovation in Instrumentation and Sample Preparation .....	639-644
Metabolomics: Targeted and Quantitative Analysis II .....	645-666
Natural Products .....	667-694
Proteins: PTMs II.....	695-715
Proteomics: Clinical Applications II.....	716-737
Proteomics: Intact Proteins and Top Down Analysis II .....	738-767
Proteomics: Quantitative II .....	768-799
Systems Biology .....	800-819

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Viruses and Virus-Like Particles .....	804-821

### AMBIENT IONIZATION: APPLICATIONS 001-020

- MP 001 **MS Imaging-Based Immunoscoring: Bringing Real-Time Intraoperative Prognosis to Life**; Léa LEDOUX<sup>1</sup>; Yanis Zirem<sup>1</sup>; Lucas Roussel<sup>1</sup>; Bertrand Meresse<sup>2</sup>; Michel Salzet<sup>1</sup>; Isabelle Fournier<sup>1</sup>; <sup>1</sup>PRISM Inserm U1192 - University of Lille, Villeneuve d'Ascq Cedex, France; <sup>2</sup>Institute for Translational Research in Inflammation (INFINITE), Lille, France
- MP 002 **Measurement of volatile PFAS from whole air and headspace using SIFT-MS**; Leslie P Silva<sup>1</sup>; Stefan J Swift<sup>2</sup>; Patrik Španěl<sup>3</sup>; Kseniya Dryahina<sup>3</sup>; Mark J. Perkins<sup>4</sup>; Vaughan S. Langford<sup>5</sup>; <sup>1</sup>Syft Technologies, Los Angeles, CA; <sup>2</sup>University of Oslo, Oslo, Norway; <sup>3</sup>J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic; <sup>4</sup>Element Lab Solutions, Cambridge, United Kingdom; <sup>5</sup>Syft Technologies, Christchurch, New Zealand
- MP 003 **Rapid Analysis of Free and Total Volatile Phenols by Sorbent Sheet Extraction-Direct Analysis in Real Time Mass Spectrometry (SPMESH-DART-MS)**; Andre P Kalenak<sup>1</sup>; Terry L Bates<sup>1, 2</sup>; Brett L Bergman<sup>1</sup>; Gavin L Sacks<sup>1</sup>; <sup>1</sup>Cornell University Dept. of Food Science, Ithaca, NY; <sup>2</sup>Bruker Daltonics Inc., Billerica, MA
- MP 004 **SICRIT-HRMS for Metabolic Profiling through Direct Breath Analysis**; Ciara Conway<sup>1, 2</sup>; Taylor Hayward<sup>3</sup>; Jan-Christoph Wolf<sup>2</sup>; Christoph Haisch<sup>1</sup>; <sup>1</sup>Technical University of Munich (TUM), Munich, Germany; <sup>2</sup>Plasmion GmbH, Augsburg, Germany; <sup>3</sup>Plasmion, Skillman, NJ
- MP 005 **Where did that come from? Non-targeted identification of micro-scale contaminants with laser desorption ionization methods**; Andre Benally<sup>1</sup>; Jessica K Kustas<sup>1</sup>; Ryan D. Davis<sup>1</sup>; <sup>1</sup>Sandia National Laboratories, Albuquerque, NM
- MP 006 **DART-MS Analysis of Antiparasitic Compounds in Bovine Hair, a powerful tool**; Almir Custódio Batista Junior<sup>1</sup>; Lanaia Louzeiro Maciel<sup>1</sup>; Yuri Arrates Rocha<sup>1</sup>; Gabriela G Souza<sup>1</sup>; Marc I Chalou<sup>2</sup>; Boniek Gontijo Vaz<sup>1</sup>; Welber Daniel Z Lopes<sup>1</sup>; Ana Flávia M. Botelho<sup>1</sup>; Andrea Rodrigues Chaves<sup>3</sup>; <sup>1</sup>Universidade Federal de Goiás, Goiânia, Brazil; <sup>2</sup>SENS Advanced Mass Spectrometry, São Paulo, Brazil; <sup>3</sup>Universidade Federal de Goiás, Goiânia, Brazil
- MP 007 **Model reference library of mass spectrometry profiles for analysis of autopsy material**; Stanislav Pekov<sup>1, 2, 3</sup>; Andrey Temnov<sup>2</sup>; Ekaterina Parochkina<sup>2</sup>; Mikhail Olfiferenko<sup>2</sup>; Olga Dorovatovskaya<sup>2</sup>; Igor Popov<sup>2, 3</sup>; <sup>1</sup>Skolkovo Institute of Science and Technology, Skolkovo, Russia; <sup>2</sup>Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; <sup>3</sup>Siberian State Medical University, Tomsk, Russia
- MP 008 **Evaluation of soft ionization by chemical reaction in transfer for the detection of small molecule organic compounds**; David Hills<sup>1</sup>; Josiah McKenna<sup>1</sup>; Connor Moreillon<sup>1</sup>; Chengli Zu<sup>1</sup>; <sup>1</sup>Corteva Agriscience, Indianapolis, IN
- MP 009 **Picosecond Infrared Laser Mass Spectrometry is sensitive to 3% brain cancer infiltration: Towards a clinically sensitive margin assessment platform**; Michael Woolman<sup>1</sup>; Lauren Katz<sup>2</sup>; Lan Anna Ye<sup>1</sup>; Georgia Gopinath<sup>2</sup>; Taira Kiyota<sup>3</sup>; Claudia Kuzan-Fischer<sup>4</sup>; Mark Zaidi<sup>2</sup>; Kaitlyn Peters<sup>2</sup>; Ahmed Aman<sup>3</sup>; Trevor McKee<sup>1</sup>; Fred Fu<sup>1</sup>; Siham Amara-Belgadi<sup>2</sup>; Craig Daniels<sup>4</sup>; Brad Wouters<sup>1</sup>; James Rutka<sup>4</sup>; Howard Ginsberg<sup>5</sup>; Chris McIntosh<sup>2</sup>; Arash Zarrine-Afsar<sup>2</sup>; <sup>1</sup>University Health Network, Toronto, ON; <sup>2</sup>University of Toronto, Toronto, ON; <sup>3</sup>Ontario Institute for Cancer Research, Toronto, ON; <sup>4</sup>The Hospital for Sick Children, Toronto, ON; <sup>5</sup>Unity Health Toronto, St Michael's Hospital, Toronto, Ontario
- MP 010 **In Situ Derivatization of Unsaturated Mid-Chain Alcohols with Pyridine during Direct Analysis in Real Time Mass Spectrometry (DART-MS)**; Zoë Scott<sup>1</sup>; Andre P Kalenak<sup>2</sup>;

## MONDAY POSTERS

- MP 011 **Portable Mass Spectrometer with Dielectric Barrier Discharge Ionization for the Direct Analysis of Controlled Substances and Explosives;** Taylor Hayward<sup>1</sup>; Krisztian Torma<sup>2</sup>; William Yang Terziyan<sup>2</sup>; Jan Bucek<sup>3</sup>; Jan-Christoph Wolf<sup>3</sup>; <sup>1</sup>Plasmion, Skillman, NJ; <sup>2</sup>BaySpec, Inc, San Jose, CA; <sup>3</sup>Plasmion GmbH, Augsburg, Germany
- MP 012 **Elucidating the Formose Reaction in aqueous microdroplets via Nano-Electrospray Ionization Mass Spectrometry;** Myles Edwards<sup>1</sup>; Dylan T. Holden<sup>2</sup>; R. Graham Cooks<sup>2</sup>; <sup>1</sup>Purdue University, West Lafayette, IL; <sup>2</sup>Purdue University Department of Chemistry, West Lafayette, IN
- MP 013 **Identification of Persistent Organic Pollutants (POPs) via Contained Electrospray Ionization (cESI);** Rebekah E Strong; *The Ohio State University, Columbus, OH*
- MP 014 **Detection of Middle Sized Synthetic Peptides by Atmospheric Pressure (AP) MALDI Mass Spectrometry;** Xiaonan Shi<sup>1</sup>; Xiaokun Duan<sup>1</sup>; Charles C. Liu<sup>1</sup>; *ASPEC Technologies, Suzhou, China*
- MP 015 **Detecting chemical threats with minimal sample preparation and without chromatographic separation;** HJ Jost<sup>1</sup>; Fariba Partovi<sup>1,2</sup>; Joonas Mikkilä<sup>1</sup>; Jyri Mikkilä<sup>1</sup>; Jussi Kontro<sup>1</sup>; Paxton Juuti<sup>1</sup>; Aleksei Shcherbinin<sup>1</sup>; <sup>1</sup>Karsa Ltd, Helsinki, Finland; <sup>2</sup>Tampere University, Tampere, Finland
- MP 016 **Direct analysis of glucose and fructose on freshly cut fruits by in-situ derivatization and ambient desorption ionization tandem mass spectrometry;** Jun J Hu<sup>1</sup>; Pingping Wang<sup>1</sup>; Lei Li<sup>1</sup>; Junliang Zhang<sup>1</sup>; <sup>1</sup>Ningbo University, Ningbo, China
- MP 017 **Rapid Screening and Quantification of PFAS in Contaminated Soil utilizing DART-MS/MS;** Zahuindanda Aventura<sup>1</sup>; Gregory Nieckarz<sup>1</sup>; <sup>1</sup>Bruker Applied Mass Spectrometry, San Jose, CA
- MP 018 **Development of Thread-Based Skin Patch for the Detection of Pulmonary Exacerbation Biomarkers in Cystic Fibrosis using Thread Spray Mass Spectrometry;** Salmika G Wairegi<sup>1</sup>; Yu Ning Shiu<sup>2</sup>; Frederick W Woodley<sup>3</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio; <sup>2</sup>The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; <sup>3</sup>Division of Gastroenterology, Hepatology and Nutrition, Nationwide Children's Hospital and The Ohio State University College of Medicine, Columbus, OH
- MP 019 **Rapid Screening of Plasma Trimethylamine N-Oxide – a Novel Risk Factor of Cardiovascular Disease with Desorption Electrospray Ionization Mass Spectrometry;** Yun-Chen Hsieh<sup>1</sup>; Hsin-Bai Zou<sup>2</sup>; Wei-Kai Wu<sup>3</sup>; Cheng-Chih Hsu<sup>1, 2</sup>; <sup>1</sup>Department of Chemistry, National Taiwan University, Taipei, Taiwan; <sup>2</sup>Leeuwenhoek Laboratories Co. Ltd., Taipei, Taiwan; <sup>3</sup>Department of Medical Research, National Taiwan University Hospital, Taipei, Taiwan
- MP 020 **Tip-Enhanced Swab Spray Ionization MS for Direct Analysis of IH Safety Swabs with Potential Toward Improved Workflows for Cleaning Verification;** John Y Kong; *Merck & Co., Inc., Rahway, NJ*
- MP 023 **Quantification of Δ9-THC and their isomers in Cannabis-based drug matrices by UHPLC-MS;** Hildegardo Seibert Franca<sup>1, 2, 3</sup>; João Victor De Almeida<sup>2, 3</sup>; Nayara A. dos Santos<sup>2, 3</sup>; Nathália Conceição<sup>2, 3</sup>; Marcos Valério V. Lyrio<sup>2, 3</sup>; Alan Reink Pereira<sup>2, 3</sup>; Wanderson Romão<sup>1, 2, 3</sup>; <sup>1</sup>Federal Institute of Espírito Santo, Brazil, Vila Velha, Brazil; <sup>2</sup>National Institute of Forensic Science and Technology, INCT, Porto Alegre, Brazil; <sup>3</sup>Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil
- MP 024 **Cross-validation of Beckman CX3 Chemistry Analyzer with Headspace Gas Chromatography-Mass Spectrometry for Measuring Total Carbon Dioxide (TCO2) in Horse Serum;** Estelle R Dowling<sup>1</sup>; Kelsey L Abbott<sup>1</sup>; Benjamin J Burris<sup>1</sup>; Soobeng Tan<sup>1</sup>; <sup>1</sup>Ohio Department of Agriculture, Reynoldsburg, OH
- MP 025 **Mass spectrometric characterization of different carbonic anhydrase isoforms: relevance in sport medicine and anti-doping analysis;** Carlotta Stacchini<sup>1</sup>; Fabio Comunità<sup>1</sup>; Xavier De La Torre<sup>1</sup>; Francesca Terracciano<sup>1</sup>; Francesco Botre<sup>1</sup>; <sup>1</sup>Laboratorio Antidoping FMSI, Roma, Italy
- MP 026 **Detection of Perfluorocarbons in Equine Blood via Headspace GC-MS/MS;** Leif K. McGoldrick<sup>1,2</sup>; Fuyu Guan<sup>1, 2</sup>; Mary A. Robinson<sup>1, 2</sup>; <sup>1</sup>Department of Clinical Studies – New Bolton Center, School of Veterinary Medicine, University of Pennsylvania, Kennett Square, PA; <sup>2</sup>Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA
- MP 027 **Multidrug Analytical Method using Polarity Switching and Scheduled MRM on the Sciex Triple Quad™ 7500 for Equine Doping Control;** Rachel Proctor<sup>1,2</sup>; Youwen You<sup>1,2</sup>; Jaclyn R. Missanelli<sup>1,2</sup>; Kacee Rossi<sup>1,2</sup>; Katelyn Stalker<sup>1,2</sup>; Mary A. Robinson<sup>1,2</sup>; <sup>1</sup>University of Pennsylvania School of Veterinary Medicine, Pennsylvania, PA; <sup>2</sup>Pennsylvania Equine Toxicology & Research Laboratory, West Chester, Pennsylvania
- MP 028 **Comprehensive analysis of minor hemp cannabinoids with therapeutic potential;** Jaewoo Choi<sup>1</sup>; Parker Rianda<sup>2</sup>; Inah Gu<sup>3, 4</sup>; Claudia S. Maier<sup>1, 3</sup>; Jan F. Stevens<sup>3, 4, 5</sup>; <sup>1</sup>Department of Chemistry, Oregon State University, Corvallis, OR; <sup>2</sup>Bioresources Research Program, College of Agricultural Sciences, Oregon State University, Corvallis, OR; <sup>3</sup>Linus Pauling Institute, Oregon State University, Corvallis, OR; <sup>4</sup>Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR; <sup>5</sup>Global Hemp Innovation Center, Oregon State University, Corvallis, OR
- MP 029 **Development of an LC-MS/MS Method for the Determination of Morphine, Oxycodone, and Hydrocodone in Human Plasma;** Alexandra M. Izydorczak<sup>1</sup>; Brandon L. Salazar<sup>2</sup>; Jill Hochreiter<sup>2</sup>; Jill Lapham<sup>2</sup>; Stephen Ross<sup>3</sup>; Troy D. Wood<sup>1</sup>; Gene D. Morse<sup>2</sup>; <sup>1</sup>Department of Chemistry, Natural Sciences Complex, University at Buffalo, State University of New York, Buffalo, NY; <sup>2</sup>Department of Pharmacy Practice, School of Pharmacy and Pharmaceutical Sciences, NYS Center for Integrated Global Biomedical Sciences, Translational Pharmacology Research Core, Buffalo, NY; <sup>3</sup>Department of Psychiatry and Child & Adolescent Psychiatry, Bellevue Hospital Center & NYU Langone Health, NYU Grossman School of Medicine, New York, NY
- MP 030 **Simultaneous detection method of muscle developing monoclonal antibodies with using LC-MS/MS from Dried Blood Spots;** Jiin Hwang<sup>1</sup>; Hyeon-Jeong Lee<sup>1</sup>; Yoodam Seo<sup>1</sup>; Hophil Min<sup>1</sup>; <sup>1</sup>Korea Institute of Science and Technology, Seoul, South Korea
- MP 031 **Simultaneous Quantitative and Exploratory Analysis of Phytocannabinoids in C. sativa Produced Locally by Brazilian Associations using the LCMS-9030;** Luis O Junqueira<sup>1</sup>; Isabel V C Fulchini<sup>2</sup>; Joice R Dos Santos<sup>2, 3</sup>; *Analysis, Cologne, Germany; <sup>3</sup>Uppsala University, Uppsala, Sweden; <sup>4</sup>University of Cologne, Cologne, Germany*

### ANTIDOPING, CANNABIS, AND OPIOID DETECTION 021-031

- MP 021 **Development and Validation of an LC-UV-HRMS Method for Identification and Quantitation of Opioid API(s) in Drug Products;** Michael Staake<sup>1</sup>; Yvonne Wu<sup>1</sup>; Brian Agan<sup>1</sup>; Jennifer Gogley<sup>1</sup>; <sup>1</sup>US Food & Drug Administration, Irvine, CA
- MP 022 **Characteristics of drug exposure scenarios in sports drug testing determined by mass spectrometry and organ-on-a-chip in-vitro and in-vivo metabolism approaches;** Mario Thevis<sup>1</sup>; Insa Peters<sup>2</sup>; Ann-Marie Garzinsky<sup>1, 3</sup>; Lina Lucuta<sup>4</sup>; Martin Juebner<sup>4</sup>; Nana Naumann<sup>2</sup>; Mikael Hedeland<sup>2</sup>; <sup>1</sup>German Sport University, Cologne, Germany; <sup>2</sup>Manfred-Donike Institute for Doping

## MONDAY POSTERS

Marcos A Pudenzi<sup>1</sup>; Diogo Oliveira-Silva<sup>2</sup>; Ichiro Hirano<sup>1</sup>; <sup>1</sup>Shimadzu do Brasil, Barueri, Brazil; <sup>2</sup>Universidade Federal de Sao Paulo, Dladema, Brazil; <sup>3</sup>Universidade de Sao Paulo, Sao Paulo, Brazil

### CARBOHYDRATES 032-040

- MP 032 **ETHcD Can Distinguish Five Co2+-Adducted Linkage and Branching Pentasaccharide Isomers**; Darren T. Gass<sup>1</sup>; Andrew M. Pritchard<sup>1</sup>; Michael S. Cordes<sup>1</sup>; Elyssia S Gallagher<sup>1</sup>; <sup>1</sup>Baylor University, Waco, TX
- MP 033 **Using High Resolution Ion Mobility for the separation and identification of α-Gal containing glycans from their non-α-Gal isomers**; Hoang Kim Ngan Thai<sup>1</sup>; Ron Orlando<sup>2</sup>; <sup>1</sup>University of Georgia - Complex Carbohydrate Research Center, Athens, GA; <sup>2</sup>Complex Carbohydrate Research Center, Department of Biochemistry and Molecular Biology, University of Georgia, Athens, GA
- MP 034 **Glycan Structural Analysis of Complex Biological Samples using a Library of Glycan Standards**; Lauren E. Pepi<sup>1, 2</sup>; Christopher Ashwood<sup>1, 2, 3</sup>; Lukas Muerner<sup>1, 4</sup>; Richard D. Cummings<sup>1, 2</sup>; <sup>1</sup>Beth Israel Deaconess Medical Center, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>Protea Glycosciences, Sydney, Australia; <sup>4</sup>University of Bern, Bern, Switzerland
- MP 035 **High Mass Range Orbitrap FTMS Imaging of Glycomic Profiles in a Syrian golden hamster model of SARS-CoV-2 variant infections**; Kayla Adcock<sup>1</sup>; Zachary Hartman<sup>1</sup>; Anton N. Kozhinov<sup>2</sup>; Konstantin Nagornov<sup>2</sup>; Eric Lafontaine<sup>1</sup>; Jeff Hogan<sup>1</sup>; Daniel G Mead<sup>1</sup>; Yury Tsybin<sup>2</sup>; Franklin E. Leach III<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Spectroswiss, Lausanne, Switzerland
- MP 036 **From Fragments to Frameworks: Characterization of Marine Polysaccharide Structures using MS-based Multi-Platforms**; Nari Seo<sup>1, 2</sup>; Hyun Joo An<sup>1, 2</sup>; <sup>1</sup>Chungnam National University, Daejeon, South Korea; <sup>2</sup>Asia-Pacific Glycomics Reference Site, Daejeon, South Korea
- MP 037 **Distinguishing Co2+-Adducted Anomeric Carbohydrate Isomers with HCD, ETD, and ETHcD**; Andrew Pritchard<sup>1</sup>; Darren T. Gass<sup>1</sup>; Elyssia S Gallagher<sup>1</sup>; <sup>1</sup>Baylor University, Waco, TX
- MP 038 **Capillary Zone Electrophoresis - Mass Spectrometry and Statistics Analysis of Plasma Chondroitin Sulphate Oligosaccharides in Septic Patients**; Yiqing Zhang<sup>1</sup>; I. Jonathan Amster<sup>2</sup>; <sup>1</sup>University of Georgia, Department of Chemistry, Athens, GA; <sup>2</sup>University of Georgia, Athens, GA
- MP 039 **Development of High Sensitivity MS Methods for Identification and Quantification of Glycosphingolipids (GSLs)**; Mehrnoush Taherzadeh Ghahfarrokhi<sup>1</sup>; Stephanie Archer-Hartmann<sup>1</sup>; Christian Heiss<sup>1</sup>; Parastoo Azadi<sup>1</sup>; <sup>1</sup>Complex Carbohydrate Research Center, University of Georgia, Athens, GA
- MP 040 **Characterizing Simple Carbohydrates Using Drift Tube and Structures for Lossless Ion Manipulations Ion Mobility for Oligomer Packing and Isomeric Resolution**; Kimberly C. Fabijanczuk<sup>1</sup>; Alexander E. Toler<sup>1</sup>; Jody C. May<sup>1</sup>; John A. McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN

### DATA-INDEPENDENT ACQUISITION 041-073

- MP 041 **Application of a non-target variable data independent workflow (vDIA) for the screening of prohibited substances in equine doping control testing**; Koon Lam Poon<sup>1</sup>; Yat Ming So<sup>1</sup>; Fred K. W. Kong<sup>1</sup>; David K. K. Leung<sup>1</sup>; April S. Y. Wong<sup>1</sup>; Wai Him Kwok<sup>1</sup>; Terence S. M. Wan<sup>1</sup>; Emmie N. M. Ho<sup>1</sup>; <sup>1</sup>Racing Laboratory, The Hong Kong Jockey Club, Sha Tin Racecourse, Sha Tin, N. T., Hong Kong, China, Hong Kong, China, Hong Kong
- MP 042 **Comprehensive phosphoproteome mapping of the macrophage response to toll-like receptor 4 stimulation using data-independent acquisition method**; Sung Hwan Yoon<sup>1</sup>; Doeun Kim<sup>1</sup>; Gwang Bin Lee<sup>2</sup>; Ling Hao<sup>2</sup>; Aleksandra

- Nita-Lazar<sup>1</sup>; <sup>1</sup>NIH/NIAID, Bethesda, MD; <sup>2</sup>The George Washington University, Washington, DC
- MP 043 **Pushing the boundaries of sensitivity and depth-of-coverage for nanoflow proteomics**; Katherine Tran<sup>1</sup>; Ihor Batruch<sup>1</sup>; Stephen Tate<sup>1</sup>; Patrick Pribil<sup>1</sup>; <sup>1</sup>SCIEX, Concord, ON
- MP 044 **SWATH-MS analysis of butyric acid effect on mAbs production and redox homeostasis in CHO cells**; Mauro Galli<sup>1</sup>; Yee Jiun Kok<sup>1</sup>; Xuezhi Bi<sup>1, 2, 3</sup>; <sup>1</sup>A-Star, Bioprocessing Technology Institute, Singapore, Singapore; <sup>2</sup>Duke-NUS Medical School, Singapore, Singapore; <sup>3</sup>Singapore Institute of Technology, Singapore, Singapore
- MP 045 **Targeted quantitative screening pesticides in food matrices using high resolution DIA spectral library matching**; Alan Barnes<sup>1</sup>; Raquel Leonardo<sup>2</sup>; Emily G Armitage<sup>1</sup>; Jonathan McGeehan<sup>3</sup>; Steve Williams<sup>2</sup>; Neil J Loftus<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Manchester, United Kingdom; <sup>2</sup>SGS Cambridge Limited, Cambridge, United Kingdom; <sup>3</sup>Shimadzu UK Limited, Milton Keynes, United Kingdom
- MP 046 **narrowPASEF: Optimized diaPASEF methods for improved differential analysis on extremely low amounts, down to single cell level**; Jeewan Babu RIJAL<sup>1</sup>; Pauline Perdu-Alloy<sup>1</sup>; Charline Keller<sup>1</sup>; Christine Schaeffer<sup>1</sup>; Christine Carapito<sup>1</sup>; <sup>1</sup>Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, UMR 7178, ProFI FR2048, CNRS Université de Strasbourg, Strasbourg, France
- MP 047 **Benchmarking informatics workflows for high-throughput and low-input proteomics analysis based on data-independent acquisition**; Zhichang Yang<sup>1</sup>; Hem Gurung<sup>2</sup>; Amanda Lorentzian<sup>2</sup>; Fengchao Yu<sup>3</sup>; Meena Choi<sup>2</sup>; Ying Zhu<sup>2</sup>; <sup>1</sup>Genentech Inc., South San Francisco, CA; <sup>2</sup>Genentech Inc, South San Francisco, CA; <sup>3</sup>University of Michigan, Ann Arbor, Michigan
- MP 048 **Differential proteomic analysis of microplastic toxicity in mouse liver by SWATH-based mass spectrometry**; Pei Chen Lin<sup>1</sup>; Sung-Fang Chen<sup>2</sup>; <sup>1</sup>National Taiwan Normal University, Taipei, Taiwan; <sup>2</sup>National Taiwan Normal University, Taipei, Taiwan
- MP 049 **Protein Quantification Assessment of diaPASEF Mode on timsTOF SCP**; Ju Wang<sup>1</sup>; Haiyan Tan<sup>1</sup>; Yingxue Fu<sup>1</sup>; Ashutosh Mishra<sup>1</sup>; Huan Sun<sup>1</sup>; Zhen Wang<sup>1</sup>; Zhiping Wu<sup>1</sup>; Xusheng Wang<sup>1</sup>; Junmin Peng<sup>1</sup>; Anthony High<sup>1</sup>; <sup>1</sup>St.Jude Children's Research Hospital, Memphis, TN
- MP 050 **High-throughput high-resolution data-independent acquisition workflow on an Orbitrap Exploris 480 Hybrid mass spectrometer for accurate label-free quantitation**; Kevin Yang<sup>1</sup>; Julia Kraegenbring<sup>2</sup>; Julian Saba<sup>3</sup>; Maciej Bromirski<sup>4</sup>; Amirmansoor Hakim<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific GmbH, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific, Winnipeg, MB; <sup>4</sup>Thermo Fisher Scientific, Warsaw, Poland
- MP 051 **Mzion-2.0: Deep Characterization of Peptides and Proteins in Data-Dependent and Independent Acquisition Mass Spectrometry**; Qiang Zhang; Washington University School of Medicine, St. Louis, MO
- MP 052 **Improving speed, sensitivity, accuracy, and comprehensiveness of covalent small molecule screening through data-independent acquisition**; Bryan Fonslow<sup>1</sup>; Sebastian V Jacome<sup>2</sup>; Nhi Ngo<sup>1</sup>; Radu M Suci<sup>1</sup>; Matthew Willetts<sup>3</sup>; Micah J Niphakis<sup>1</sup>; <sup>1</sup>Lundbeck, San Diego, CA; <sup>2</sup>Bruker Scientific, 40 Manning Road, Billerica, MA; <sup>3</sup>Bruker Scientific, LLC, Billerica, MA
- MP 053 **Deep Proteomic Profiling of Accelerated Kidney Aging and Senescence Burden in Macaca mulatta**; Christina D King<sup>1</sup>; Jordan B Burton<sup>1</sup>; George Schaa<sup>2</sup>; Stephen Kritchevsky<sup>2</sup>; J. Mark Cline<sup>2</sup>; Jamie N Justice<sup>2, 3</sup>; Ellen E Quillen<sup>2</sup>; Birgit Schilling<sup>1</sup>; <sup>1</sup>Buck Institute for Research on Aging, Novato, CA; <sup>2</sup>Wake Forest University School of Medicine, Winston-Salem, NC; <sup>3</sup>XPRIZE Foundation, Culver City, CA

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- MP 054 **Database search result comparison for Spectronaut and DIANN for DIA data collected from QE, Fusion, Eclipse, Exploris and TimsTOF Pro2;** Dennis Province<sup>1</sup>; Stephanie Byrum<sup>1</sup>; Michael Kinter<sup>2</sup>; Ricky Edmondson<sup>1</sup>; Samuel Mackintosh<sup>1</sup>; Alan Tackett<sup>1</sup>; <sup>1</sup>UAMS, Little Rock, AR; <sup>2</sup>Oklahoma Medical Research Foundation, Oklahoma City, Oklahoma
- MP 055 **Improved proteome coverage combined with reproducible quantitation on the timsTOF platform;** Dijana Vitko<sup>1</sup>; Stephanie Kaspar-Schoenefeld<sup>2</sup>; Andreas Schmidt<sup>2</sup>; Markus Lubeck<sup>2</sup>; Pierre-Olivier Schmit<sup>3</sup>; Torsten Mueller<sup>2</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Billerica, MA; <sup>2</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>3</sup>Bruker France SAS, Wissembourg, France
- MP 056 **A scanning DIA workflow for quantitative LC-MS/MS with minimal method development;** Anjali Chelur<sup>1</sup>; Gordana Ivosev<sup>1</sup>; Nic G Bloomfield<sup>1</sup>; Claudia Alvarez<sup>1</sup>; Stephen Tate<sup>1</sup>; <sup>1</sup>SCIEX, Concord, ON
- MP 057 **Synchronizing analysis with acquisition for significantly faster library free analysis of DIA;** Damiano Robbiani<sup>1</sup>; Grzegorz Skoraczynski<sup>1</sup>; Oliver M. Bernhardt<sup>1</sup>; Tejas Gandhi<sup>1</sup>; Lukas Reiter<sup>1</sup>; <sup>1</sup>Biognosys AG, Schlieren, Switzerland
- MP 058 **High-throughput cancer proteomic characterization using data-independent mass spectrometry (DIA-MS);** Chih-Hsuan Yeh<sup>1, 2</sup>; Sebastian P. Perner<sup>1, 3</sup>; Yanlong Ji<sup>1, 2</sup>; Silvia Münch<sup>3</sup>; Thomas Oellerich<sup>3</sup>; Kuan-Ting Pan<sup>1</sup>; Henning Urlaub<sup>1, 2</sup>; <sup>1</sup>Bioanalytical Mass Spectrometry Group, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; <sup>2</sup>Bioanalytics Group, Institute of Clinical Chemistry, University Medical Center Göttingen, Göttingen, Germany; <sup>3</sup>University Hospital Frankfurt, Department of Hematology/Oncology, Frankfurt am Main, Germany
- MP 059 **High-throughput SILAC quantification using narrow width data-independent acquisition on the Orbitrap Astral Mass Spectrometer;** Tabiwang N. Arrey<sup>1</sup>; Amarjeet Flora<sup>2</sup>; Bhavin Patel<sup>2</sup>; Santosh Renuse<sup>3</sup>; Ryan Bomgarden<sup>2</sup>; Nicolaie Eugen Damoc<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific GmbH, Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific, Rockford, Illinois; <sup>3</sup>ThermoFisher Scientific, San Jose, CA
- MP 060 **Fast and Effective Quality Control in Data Independent Acquisition in Proteomic Workflows;** Taufika Islam Williams; NCSU, Raleigh, NC
- MP 061 **A comparison of peptide- and spectrum-centric search engines beyond bar charts;** Michelle Tamara Berger<sup>1</sup>; Alexander Hogrebe<sup>1</sup>; Daniel P Zolg<sup>1</sup>; Florian Seefried<sup>1</sup>; Martin Frejno<sup>1</sup>; <sup>1</sup>MSAID, Garching, Germany
- MP 062 **Trapped Ion Mobility Separation (TIMS) in Combination with Scanning Quadrupole Isolation for Data Independent Acquisition in Proteomics;** Markus Lubeck<sup>1</sup>; Eike Mucha<sup>1</sup>; Stephanie Kaspar-Schoenefeld<sup>1</sup>; Christoph Krisp<sup>1</sup>; Andreas Schmidt<sup>1</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- MP 063 **DIA analysis of Nrf2 and  $\alpha$ B-crystallin mutant zebrafish lenses under oxidative stress;** Sarah Zelle<sup>1</sup>; Hassane S. Mchaourab<sup>1</sup>; Kevin L. Schey<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- MP 064 **Quantitative and Qualitative Evaluation Performance of diaPASEF for Targeted Protein Degradation;** Duc Tran<sup>1</sup>; Shu You<sup>1</sup>; Alex Campos<sup>1</sup>; <sup>1</sup>Plexium, San Diego, CA
- MP 065 **Quantifying the Benefits of Using Study-Specific Data-Independent Acquisition Libraries for Proteomics Analysis;** Mynaja Ferguson<sup>1</sup>; Dorianne Robasson<sup>2</sup>; Rachel Muriph<sup>1</sup>; Kai Zou<sup>1</sup>; Hannah Rosen<sup>2</sup>; Jason Evans<sup>2</sup>; <sup>1</sup>University of Massachusetts Boston, Boston, MA; <sup>2</sup>University of Massachusetts Boston, Boston, MA
- MP 066 **Direct, spectrum-centric peptide identification from diaPASEF data;** Kai Li<sup>1</sup>; Fengchao Yu<sup>1</sup>; Alexey I. Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, Michigan
- MP 067 **Data independent acquisition (DIA) for peptide library generation prior to HDX-MS;** Oliver Wu<sup>1</sup>; Joel B Langford<sup>1</sup>; Kellye Cupp-Sutton<sup>2</sup>; Nathan Basisty<sup>3</sup>; Si Wu<sup>2</sup>; <sup>1</sup>University of Oklahoma, Norman, OK; <sup>2</sup>University of Alabama, Tuscaloosa, AL; <sup>3</sup>National Institute on Aging, National Institutes of Health, Baltimore, MD 21224
- MP 068 **Optimizing DIA-PASEF with Sample-Specific Ion Mobility for Enhanced Deep Proteomics Analysis;** Raghothama Chaerkady<sup>1</sup>; Morgan Fair<sup>1</sup>; Liang Zhao<sup>1</sup>; Qing Wang<sup>1</sup>; <sup>1</sup>CompleteOmics, Halethorpe, MD
- MP 069 **Cross-instrument, multi-step assessment and optimization of plex-DIA quantifying selective protein turnover under genome dosage imbalance;** Barbora Salovska<sup>1</sup>; Wenxue Li<sup>1</sup>; Yi Di<sup>1</sup>; Diego Assis<sup>2</sup>; Matthew Willetts<sup>2</sup>; Yansheng Liu<sup>1</sup>; <sup>1</sup>Yale University, West Haven, CT; <sup>2</sup>Bruker life sciences, Billerica, MA
- MP 070 **Evaluating mass spectrometry strategies for deep proteome profiling with subcellular fractionation;** Andrea I Gutierrez<sup>1</sup>; Julia E Robbins<sup>1</sup>; J. Sebastian Paez<sup>1</sup>; Tonibelle Gatbonton-Schwager<sup>1</sup>; Alexander J Federation<sup>1</sup>; Daniele Canzani<sup>1</sup>; Lindsay K Pino<sup>1</sup>; <sup>1</sup>Talus Bioscience, Seattle, WA
- MP 071 **Unraveling Mechanisms of Cisplatin Resistance via DIA-based Proteomics and Expanding the Horizons of Omics-Driven Drug Repurposing in Squamous Cervix Carcinoma;** Amrita Mukherjee<sup>1</sup>; Avinash Singh<sup>1</sup>; Sanjeeva Srivastava<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Bombay, Mumbai, India
- MP 072 **Building a Comprehensive, Quantitative Library of Placenta Transporters Throughout Development Using Data-Independent Analysis and MRM Proteomics;** Eric M Weaver<sup>1</sup>; Samuel L Arnold<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- MP 073 **High-throughput high-resolution data-independent acquisition workflow on an Orbitrap Ascend Tribrid mass spectrometer for accurate label-free quantitation;** Kevin Yang<sup>1</sup>; Julia Kraegenbring<sup>2</sup>; Julian Saba<sup>3</sup>; Amanda E Lee<sup>4</sup>; Tonya Pekar-Hart<sup>1</sup>; Jingjing Huang<sup>1</sup>; Amirmansoor Hakimi<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific, Winnipeg, MB; <sup>4</sup>Thermo Fisher Scientific, Worcester, MA

### DRUG DISCOVERY / DMPK / ADME 074-098

- MP 074 **Developing a Targeted LC-HRMS Workflow for Quantifying Transporter Proteins in Complex In-vitro System;** Dangqing Wang<sup>1</sup>; Yusi Cui<sup>1</sup>; Yuling Dai<sup>2</sup>; Benjamin Lai<sup>1</sup>; Qinying Yu<sup>1</sup>; Eugene Chen<sup>1</sup>; Xing Zhang<sup>1</sup>; <sup>1</sup>Genentech Inc, South San Francisco, CA; <sup>2</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin
- MP 075 **LC/MS/MS characterization of novel lipid metabolism for mRNA therapeutics & vaccines;** Ashish Vaswani<sup>1</sup>; Christopher Rowbottom<sup>1</sup>; John Wickwire<sup>1</sup>; Mark Brader<sup>1</sup>; Ling Morgan<sup>1</sup>; <sup>1</sup>Moderna, Cambridge, MA
- MP 076 **Identifying and Assessing Target Engagement of Ligands Binding to Activin Ligand Traps;** Mark Athanason<sup>1</sup>; Keun-Joong Lee<sup>1</sup>; Matthew Mazur<sup>1</sup>; Yan Gao<sup>1</sup>; Richard Chen<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., Rahway, NJ, USA, Rahway, NJ
- MP 077 **In vitro and in vivo metabolism of anti-SARS-CoV-2 agent 1'-cyano-cytidine;** Sijia Tao<sup>1</sup>; Franck Amblard<sup>1</sup>; Selwyn Hurwitz<sup>1</sup>; Mahesh Kasthuri<sup>1</sup>; Chengwei Li<sup>1</sup>; Julia LeCher<sup>1</sup>; Junxing Shi<sup>1</sup>; Ramyani De<sup>1</sup>; Jessica Bowen-Downs<sup>1</sup>; Raymond Schinazi<sup>1</sup>; <sup>1</sup>Emory University School of Medicine, Atlanta, GA
- MP 078 **Combining In Vitro Metabolism and Whole-Body Biodistribution for Comprehensive Insight into ERAP2 inhibitor Pharmacokinetic;** Adele-Asia Ponzoni<sup>1, 2</sup>; Nour Bou Karroum<sup>3</sup>; Catherine Piveteau<sup>3</sup>; Aurore Tomezyk<sup>1</sup>; Julie Dumont<sup>3</sup>; Mathieu Gaudin<sup>1</sup>; Rebecca Deprez-Poulain<sup>2, 3</sup>; Corinne Ramos<sup>1, 2</sup>; Benoit Deprez<sup>3</sup>; <sup>1</sup>Aliri, Loos, France; <sup>2</sup>CAPSTONE-ETN MSCA network, Lille, France; <sup>3</sup>Drugs and Molecules for Living Systems, U1177, Lille, France
- MP 079 **Accurate Identification of Phase I Oxidative Metabolites of the Proteolysis Targeting Chimeras (PROTAC™)**

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- MP 080 **Degrader GNE-987; Pengyi Hou<sup>1</sup>; Dandan Si<sup>1</sup>; Zhimin Long<sup>1</sup>; Lihai Guo<sup>1</sup>; <sup>1</sup>SCIEX, Beijing, China**  
**Enhancement of Sensitivity and Quantification Quality in the LC-MS/MS Measurement of Large Biomolecules with Sum of MRM (SMRM); Liang Tang<sup>1</sup>; Robert R. Swezey<sup>1</sup>; Carol E. Green<sup>1</sup>; Jon C. Mirsalis<sup>1</sup>; <sup>1</sup>SRI International, Menlo Park, CA**
- MP 081 **Labeling of lipopeptides with lanthanide tag enables their monitoring in biological tissues by ICP-MS; Aneta Myskova<sup>1,2</sup>; Antonín Kaňka<sup>1</sup>; Tomáš David<sup>2</sup>; David Sýkora<sup>1</sup>; Miloslav Polášek<sup>2</sup>; Miroslava Šedinová<sup>2</sup>; Jaroslav Kuneš<sup>3</sup>; Lenka Maletínská<sup>2</sup>; <sup>1</sup>University of Chemistry and Technology Prague, Prague, Czech Republic; <sup>2</sup>Institute of Organic Chemistry and Biochemistry, CAS, Prague, Prague, Czech Republic; <sup>3</sup>Institute of Physiology, CAS, Prague, Prague, Czech Republic**
- MP 082 **Quality on the Clock: Rapid QC of LC-MS Data for Discovery PK; Christopher B. Lietz<sup>1</sup>; Sarah Franc<sup>1</sup>; Bocheng Yin<sup>1</sup>; Fletcher Paddison<sup>1</sup>; Gyana Cureg<sup>1</sup>; Fabio Broccatelli<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb, San Diego, CA**
- MP 083 **Comprehensive Workflow for Quantitative Bioanalysis of Large Peptides and Proteins: Case Study of GLP-1 Receptor Agonist Semaglutide in Plasma; Samantha Ferries<sup>1</sup>; Suraj Dhungana<sup>2</sup>; Robert Plumb<sup>2</sup>; Amy Bartlett<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Waters, Milford, MA**
- MP 084 **Investigation of the pharmacokinetic properties of PEGylated bilirubin in rats after subcutaneous administration using liquid chromatography-quadrupole time-of-flight mass spectrometry; Seo-jin Park<sup>1</sup>; Jeong-hyeon Lim<sup>1</sup>; Sangsoo Hwang<sup>1</sup>; Yuna Shin<sup>2</sup>; Hyunjin Kim<sup>2</sup>; Seunghyun Jo<sup>2</sup>; Duckhyang Shin<sup>2</sup>; Sang Ho MA<sup>2</sup>; Myung L. Kim<sup>2</sup>; Young G. Shin<sup>1</sup>; <sup>1</sup>College of Pharmacy and Institute of Drug Research and Development, Chungnam National University, Daejeon, South Korea; <sup>2</sup>Bilix Co., Ltd., Yongin, South Korea**
- MP 085 **Bioanalytical Method Development and its Application to Pharmacokinetic Characterization of Tramiprosate and ALZ-801; Jeonghyeon Lim<sup>1</sup>; Jeongmin Lee<sup>2</sup>; Seo-jin Park<sup>2</sup>; Sang-soo Hwang<sup>2</sup>; Eun-jeong Jo<sup>2</sup>; Young G. Shin<sup>2</sup>; <sup>1</sup>Chungnam National University, Daejeon, South Korea; <sup>2</sup>Chungnam National University, Daejeon, South Korea**
- MP 086 **Design of Estrogen-Like Molecules with a Potential to Improve Brain Penetration for an Enhanced Memory in Ovariectomized Mouse Model; Julien Breault-Turcot<sup>1</sup>; Annie Run Qi Shao<sup>1</sup>; Linh Nguyen<sup>1</sup>; Harun Rashid<sup>1</sup>; William Donaldson<sup>2</sup>; <sup>1</sup>NuChem Sciences Inc., Montréal, QC; <sup>2</sup>Estrigenix Therapeutics, Milwaukee, WI**
- MP 087 **Utilization of CID and EAD fragmentation for metabolite identification in three hepatocyte models; Yiran Huang<sup>1</sup>; Bennett K Ma<sup>1</sup>; Amy G Aslamkhan<sup>1</sup>; <sup>1</sup>Merck Sharp & Dohme LLC, West Point, PA**
- MP 088 **Ultra-Performance Liquid Chromatography-Tandem Mass Spectrometry Method Development and Pharmacokinetics of 10 $\beta$ ,17 $\beta$ -Dihydroxyestra-1,4-dien-3-one (DHED) in Mice; Amy Q Wang<sup>1</sup>; China Ryu<sup>1</sup>; Elias Padilha<sup>1</sup>; Patrick J. Morris<sup>1</sup>; Abigail F Postle<sup>2</sup>; Chris F Powels<sup>2</sup>; Todd D Gould<sup>2</sup>; Xin Xu<sup>1</sup>; <sup>1</sup>NIH, Rockville, MD; <sup>2</sup>University of Maryland, Baltimore, MD**
- MP 089 **Investigating a Novel Bioanalytical Approach for Monoclonal Antibodies in Brain Tissue via Immunoprecipitation and Liquid Chromatography-Mass Spectrometry; Sangsoo Hwang<sup>1</sup>; Seo-jin Park<sup>1</sup>; Jeong-hyeon Lim<sup>1</sup>; Young G. Shin<sup>1</sup>; <sup>1</sup>College of Pharmacy and Institute of Drug Research and Development, Chungnam National University, Daejeon, South Korea**
- MP 090 **Definitive Identification of Cyclic Peptide Soft Spot by Reductive Dimethylation and Mass Spectrometry Fragmentation; Athanasia Qirjollari<sup>1</sup>; Maria Fawaz<sup>1</sup>; Mark T. Cancelli<sup>1</sup>; Raymond Gonzalez<sup>1</sup>; Kara M Pearson<sup>1</sup>; Yu Feng<sup>1</sup>; <sup>1</sup>Merck & Co. Inc., West Point, PA**
- MP 091 **Beyond Western Blot: LC-MS Revolutionizes Protein Analysis with Speed and Precision; Dhaval Patel<sup>1</sup>; Yash Mehta<sup>1</sup>; Ulrich Bickel<sup>1</sup>; Abraham Al-Ahmad<sup>1</sup>; <sup>1</sup>Texas Tech University Health Sciences Center, Amarillo, TX**
- MP 092 **Evaluation of BioMimetic Oxidation Kit for Fast and Efficient Abiotic Metabolite Generation; Rong Chen<sup>1</sup>; Vivek Badwaik<sup>1</sup>; Jesse Balcer<sup>1</sup>; Chengli Zu<sup>1</sup>; <sup>1</sup>Corteva Agriscience, Indianapolis, IN**
- MP 093 **Proteomic-Based Site-Specific Covalent Ligand Screening for FBDD-Driven PROTAC Development Targeting MDM2; Hyeonjun Lee<sup>1</sup>; Ju Yeon Lee<sup>2</sup>; Minhee Kang<sup>1</sup>; Suin Kim<sup>1</sup>; Jaebong Jang<sup>1</sup>; Jin Young Kim<sup>2</sup>; Young Ho Jeon<sup>1</sup>; <sup>1</sup>College of Pharmacy, Korea University, Sejong, South Korea; <sup>2</sup>Korea Basic Science Institute, Ochang, South Korea**
- MP 094 **Target Identification of a Novel Small Molecule Autophagy Modulator Through Proteomics; Zi Gao; Scripps Research, San Diego, CA**
- MP 095 **Sensitive bioanalysis method for antisense oligonucleotides using LC-MS/MS; Lee Bertram; Agilent Technologies, Santa Clara, CA**
- MP 096 **Evaluating Fc modifications and molecular formats on neonatal Fc receptor binding using affinity-resolved size exclusion chromatography coupled to mass spectrometry; Tao Xing<sup>1</sup>; Yuetian Yan<sup>1</sup>; Shunhai Wang<sup>1</sup>; Ning Li<sup>1</sup>; <sup>1</sup>Regeneron Pharmaceuticals Inc., Tarrytown, NY**
- MP 097 **Implementation Study: Quantitative Tuneless High Resolution LC/MS workflows for improved assay productivity and success for ADME permeability studies; Emile Plise<sup>1</sup>; Loren Olson<sup>2</sup>; Jamie Jorski<sup>1</sup>; Christopher Chhin<sup>1</sup>; Wayne Lootsma<sup>3</sup>; Steve Ainley<sup>3</sup>; Jeremy Lawton<sup>3</sup>; Laurent Salphati<sup>1</sup>; <sup>1</sup>Genentech Inc, South San Francisco, CA; <sup>2</sup>SCIEX, Redwood City, CA; <sup>3</sup>Sound Analytics, Deep River, CT**
- MP 098 **Leveraging Low Micro- and Nanoflow LC-MS/MS for Small Molecule Bioanalysis; Christopher Healy; Pfizer, Groton, CT**

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- MP 099 **Electron Activated Dissociation (EAD) for elucidating the structures of synthetic small molecules; Shuai Wu<sup>1</sup>; Jeffrey J. Jacson<sup>1</sup>; Iain D.G. Campuzano<sup>1</sup>; Rahul Baghla<sup>2</sup>; <sup>1</sup>Amgen Inc., Thousand Oaks, CA; <sup>2</sup>SCIEX, Redwood City, CA**
- MP 100 **Doping Control of Estra-4,9-diene-3,17-dione in horses; Helen S.M. Ho<sup>1</sup>; Adrian F. Farrington<sup>2</sup>; Amanda J. Bond<sup>3</sup>; Emmie N. M. Ho<sup>1,4</sup>; Wing-Tak Wong<sup>1</sup>; <sup>1</sup>The Hong Kong Polytechnic University, Hong Kong, Hong Kong; <sup>2</sup>Department of Veterinary Clinical Services, The Hong Kong Jockey Club, Sha Tin Racecourse, Sha Tin, N. T., Hong Kong, China, Hong Kong, China, Hong Kong; <sup>3</sup>Equestrian Affairs, The Hong Kong Jockey Club, Sha Tin Racecourse, Sha Tin, N. T., Hong Kong, China, Hong Kong, China, Hong Kong; <sup>4</sup>Racing Laboratory, The Hong Kong Jockey Club, Sha Tin Racecourse, Sha Tin, N. T., Hong Kong, China, Hong Kong, China, Hong Kong**
- MP 101 **LC/HRMS analysis for documenting the Production of Fungal Perylenequinones by fungi grown under different conditions; Reema Al-Qiam<sup>1</sup>; Firoz Khan<sup>1</sup>; Huzefa Raja<sup>1</sup>; Cedric Pearce<sup>2</sup>; Shabnam Hematian<sup>1</sup>; Nicholas Oberlies<sup>1</sup>; <sup>1</sup>UNCG, Greensboro, NC; <sup>2</sup>Mycosynthetix, Inc., Greensboro, North Carolina**
- MP 102 **In vitro and in vivo biotransformation assessment of PEGylated lipids in lipid nanoparticles with LC-Orbitrap high resolution mass spectrometry; Peng Li<sup>1</sup>; Ya Ding<sup>1</sup>; Lian Guo<sup>1</sup>; Lingling Zhang<sup>1</sup>; Weiqun Cao<sup>1</sup>; Yi Tao<sup>1</sup>; Liang Shen<sup>1</sup>; <sup>1</sup>DMPK Service Department, Lab Testing Division, WuXi AppTec, Nanjing, China**
- MP 103 **Characterizing glutathione adduct using feature-based molecular networking combined with multivariate analysis; Young-Heun Jung<sup>1</sup>; Ju-Hyun Kim<sup>1</sup>; <sup>1</sup>Yeungnam University, Gyeongsan-si, South Korea**



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- MP 104 **Elucidation of Isomeric Metabolites of Cyclic Peptide Pharmaceuticals Using HPLC/ESI-Exact-Mass-MS/MS Data with MASSPEC Structure Elucidation Software;** Marshall M. Siegel<sup>1</sup>; Serhiy Hnatyshyn<sup>2</sup>; Gary Walker<sup>1</sup>; <sup>1</sup>MS Mass Spec Consultants, Fair Lawn, NJ; <sup>2</sup>Bristol-Meyers Squibb, Princeton, NJ, Princeton, NJ
- MP 105 **A Novel LC-MS/MS Method for the Determination of Thiocyanate in Human Plasma;** Christina Chang<sup>1</sup>; Donald Chun<sup>1</sup>; Veronica Viramontes<sup>1</sup>; Zhili Li<sup>1</sup>; David Cipolla<sup>1</sup>; <sup>1</sup>Insmad, Bridgewater Township, NJ
- MP 106 **Metabolite identification of the targeted protein degrader, ARV-110;** Junmiao Chen<sup>1</sup>; Dandan Si<sup>1</sup>; Zhimin Long<sup>1</sup>; Lihai Guo<sup>1</sup>; <sup>1</sup>SCIEX, Beijing, China
- MP 107 **Benefits of DIA for metabolism studies;** Stephen Tate<sup>1</sup>; Chris Brown<sup>2</sup>; Jeffrey R Gilbert<sup>2</sup>; Yves LeBlanc<sup>1</sup>; <sup>1</sup>SCIEX, Concord, ON; <sup>2</sup>Corteva Agriscience, Indianapolis, IN
- MP 108 **Novel stereoselective reversed-phase LC-MS method for quantification of 9R- and 9S-hexahydrocannabinols in biological matrices;** Lucie Janeckova<sup>1</sup>; Magdalena Vagnerova<sup>2, 3</sup>; Monika Mrnava<sup>1</sup>; Petr Palivec<sup>1</sup>; Martin Kuchar<sup>1</sup>; <sup>1</sup>Forensic Laboratory of Biologically Active Substances, Department of Chemistry of Natural Compounds, University of Chemistry and Technology Prague, Prague 6, Czech Republic; <sup>2</sup>Forensic Laboratory of Biologically Active Substances, Department of Chemistry of Natural Compounds, University of Chemistry and Technology, Prague, Czech Republic; <sup>3</sup>Department of Analytical Chemistry, University of Chemistry and Technology Prague, Prague 6, Czech Republic
- MP 109 **Investigating the metabolism of an Antibody-siRNA conjugate in vitro and in vivo using a complementary set of untargeted LC-HRMS methods;** Christophe Husser<sup>1</sup>; Felix Schumacher<sup>1</sup>; Kerstin Hofer<sup>2</sup>; Mads Mansoe<sup>3</sup>; Christian Weile<sup>3</sup>; Erich Koller<sup>1</sup>; Sabine Lohmann<sup>2</sup>; Sabine Schuster<sup>2</sup>; Andreas Brink<sup>1</sup>; <sup>1</sup>Pharma Research and Early Development, Roche Innovation Center Basel, Basel, Switzerland; <sup>2</sup>Pharma Research and Early Development, Roche Innovation Center Munich, Penzberg, Germany; <sup>3</sup>Pharma Research and Early Development, Roche Innovation Center Copenhagen, Hørsholm, Denmark
- MP 110 **LC-MS/MS Based In-vitro Metabolic Profiling of Natural Cyclic-Diarylheptanoid in Rat Liver Microsomes;** A. F. M. Motiur Rahman<sup>1</sup>; Wencui Yin<sup>1</sup>; Adnan A Kadi<sup>1</sup>; <sup>1</sup>King Saud University, Riyadh, Saudi Arabia
- MP 111 **High-Throughput Screening and Proteomic Characterization of Compounds Targeting Myeloid-Derived Suppressor Cells;** Johannes Krumm<sup>1, 2</sup>; Elissaveta Petrova<sup>3</sup>; Severin Lechner<sup>2</sup>; Julia Mergner<sup>2</sup>; Hans-Henning Boehm<sup>3</sup>; Alessandro Prestipino<sup>3</sup>; Dominik Steinbrunn<sup>1</sup>; Marshall L. Deline<sup>4</sup>; Hannes Hahne<sup>1</sup>; Jan-Carsten Piek<sup>3</sup>; Bernhard Kuster<sup>2</sup>; <sup>1</sup>OmicScouts GmbH, Freising, Germany; <sup>2</sup>Chair of Proteomics and Bioanalytics, TU Munich, TUM School of Life Sciences, Freising, Germany; <sup>3</sup>Merck KGaA, Darmstadt, Germany; <sup>4</sup>Chair of Molecular Nutritional Medicine, TUM School of Life Sciences, Technical University of Munich, Freising, Germany
- MP 112 **High-Throughput Metabolism Simulation by LC-EC-MS and Molecular Networking;** Erik Niehaves<sup>1</sup>; Giovanni Andrea Vitale<sup>2</sup>; Steffen Heuckeroth<sup>1</sup>; Daniel Petras<sup>2, 3</sup>; Uwe Karst<sup>1</sup>; <sup>1</sup>University of Muenster, Muenster, Germany; <sup>2</sup>University of Tuebingen, CMFI Cluster of Excellence, Interfaculty Institute of Microbiology and Infection Medicine, Tuebingen, Germany; <sup>3</sup>UC Riverside, Riverside, CA
- MP 113 **Application of LC-HRMS for metabolic studies of hexahydrocannabinol (HHC) using Cunninghamella elegans mycelia and Wistar rat models ;** Monika Mrnava<sup>1</sup>; Magdalena Vagnerova<sup>1, 2</sup>; Lucie Janeckova<sup>1</sup>; Martin Kuchar<sup>1</sup>; Petr Palivec<sup>1</sup>; Bronislav Jurasek<sup>1</sup>; <sup>1</sup>Forensic Laboratory of Biologically Active Substances, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic; <sup>2</sup>Department of Analytical Chemistry, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic
- MP 114 **Confident transformation site localization of PROTAC drug metabolites facilitated by multi-stage fragmentation LC-HRAM-MS;** Sven Hackbusch<sup>1</sup>; Min Du<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Lexington, MA
- MP 115 **Simultaneous Quantitation of Prednisone and Prednisolone in Human Plasma by LC-MS/MS;** Moo-Young Kim<sup>1</sup>; Xuguang Yan<sup>1</sup>; Weijun Sun<sup>1</sup>; Zhijing Huang<sup>1</sup>; Melissa Mofikoya<sup>1</sup>; <sup>1</sup>PPD, Middleton, WI
- MP 116 **Rapid Data Rationalization for Biotransformation using a Novel Benchtop Multi-Reflecting Time-of-Flight Mass Spectrometer with Dedicated Data-Mining Software;** Daniel J Weston<sup>1</sup>; Hania Khoury-Hollins<sup>2</sup>; Ismael Zamora<sup>3</sup>; Fabien Fontaine<sup>3</sup>; Michael McCullagh<sup>2</sup>; Martin Palmer<sup>2</sup>; Richard Lock<sup>2</sup>; Laura Tomlinson<sup>1</sup>; Leah Bottomley<sup>1</sup>; Richard Gregory<sup>1</sup>; <sup>1</sup>GSK, Stevenage, United Kingdom; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>3</sup>Mass Analytica Ltd, Sant Cugat del Vallés, Spain
- MP 117 **The Automated Sample Preparation Workflow and Toolbox for Bioanalysis;** Yuan Li<sup>1</sup>; Kyle Dukes<sup>1</sup>; Amber Cain<sup>1</sup>; Esraa AboJasser<sup>1</sup>; <sup>1</sup>Biotage LLC., CLT, NC
- MP 118 **Metabolism simulation of new psychoactive substances utilizing electrochemistry-mass spectrometry: Introducing an innovative software tool for rapid data evaluation;** Mark Wesner<sup>1</sup>; Steffen Heuckeroth<sup>1</sup>; Michael Pütz<sup>2</sup>; Uwe Karst<sup>1</sup>; <sup>1</sup>University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; <sup>2</sup>Federal Criminal Police Office, Forensic Science Institute, Wiesbaden, Germany
- MP 119 **Paxlovid Unveiled: LC-MS/MS Insights onto the Pharmacokinetics of Nirmatrelvir and Ritonavir in Human Milk;** PALIKA DATTA<sup>1</sup>; Kaytlin Krutsch<sup>1</sup>; Dhavalkumar Patel<sup>1</sup>; Teresa Baker<sup>1</sup>; <sup>1</sup>Texas Tech University Health Sciences Center, Amarillo, TX
- MP 120 **An automated software-assisted approach for exploring metabolic susceptibility and degradation products in macromolecules using High-Resolution Mass Spectrometry;** Paula Cifuentes<sup>1, 2</sup>; Ismael Zamora<sup>1</sup>; Fabien Fontaine<sup>1</sup>; Albert Garriga<sup>1</sup>; Luca Moretton<sup>3</sup>; Tatiana Radchenko<sup>4</sup>; <sup>1</sup>Mass Analytica, S.L, Sant Cugat del Vallés, Spain; <sup>2</sup>Universitat Pompeu Fabra, Barcelona, Spain; <sup>3</sup>Mass Analytica, S.L, Bettona, Italy; <sup>4</sup>Lead Molecular Design, S.L, Sant Cugat del Vallés, Spain
- MP 121 **Quantitative analysis of drugs in mimetic tissue models using nano-DESI on a triple quadrupole mass spectrometer;** Alyssa Moore<sup>1</sup>; Syeda Nazifa Wali<sup>1</sup>; Miranda Weigand<sup>1</sup>; Andrew Bowman<sup>2</sup>; David Wagner<sup>2</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>AbbVie Inc., North Chicago, IL
- MP 122 **Evaluation of potential spike-in proteins for normalization of TPP quantitation;** Chunna Guo<sup>1</sup>; Katelyn Caric<sup>1</sup>; Whitney Smith-Kinnaman<sup>2</sup>; Emma H Doud<sup>2</sup>; Amber L Mosley<sup>2</sup>; <sup>1</sup>Indiana University, Indianapolis, IN; <sup>2</sup>Indiana University School of Medicine, Indianapolis, IN
- MP 123 **Microvolume quantification of amodiaquine and its metabolite desethylamodiaquine in plasma by ultra high performance liquid chromatography tandem mass spectrometry;** Florence Marzan<sup>1</sup>; Liusheng Huang<sup>2</sup>; David Gingrich<sup>1</sup>; Francesca Aweeka<sup>1</sup>; <sup>1</sup>University of California-San Francisco, San Francisco, CA; <sup>2</sup>University of California San Francisco, San Francisco, CA
- MP 124 **In vitro SR9011 metabolism study using tandem mass spectrometry;** Maxime Sansoucy<sup>1</sup>; Myriam Soucy<sup>2</sup>; Éric Morneau<sup>1</sup>; Benoit Daoust<sup>2</sup>; Simon Ricard<sup>2</sup>; Jean-François Naud<sup>1</sup>; <sup>1</sup>Doping Control Laboratory - INRS, Laval, QC; <sup>2</sup>UQTR, Trois-Rivières, QC
- MP 125 **Troubleshooting to Resolve Chromatographic Interference Observed in Human Plasma Samples using a Previously Validated LC-MS/MS method for Clarithromycin and 14-Hydroxylclarithromycin;** Xuguang Yan<sup>1</sup>; Zhijing Huang<sup>1</sup>; Moo-Young Kim<sup>1</sup>; Melissa Mofikoya<sup>1</sup>; <sup>1</sup>PPD, Middleton, WI

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- MP 126 **Continued development of a self-service LC-QTOF based metabolomics training curriculum/workflow in an open access core facility;** Paul G Mathews<sup>1</sup>; Claudia Boot<sup>1</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO
- MP 127 **Ambient ionization of small molecules: a quest between physics, chemistry, and mathematics;** Stanislav Pekov; *Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation*
- MP 128 **Modelling ion trajectories in quadrupole fields using Python. A student exercise in our undergraduate chemical instrumentation course;** Robert L McClain<sup>1</sup>; John G Pavek<sup>1</sup>; John C. Wright<sup>1</sup>; <sup>1</sup>University of Wisconsin Madison, Madison, WI
- MP 129 **To "Walk-Up" or Run Away? Starting, Maintaining, and Training Users for a Shared LC/MS Resource in a Core Facility;** Curtis Mowry<sup>1</sup>; Tyler Hipple<sup>1</sup>; <sup>1</sup>University of New Mexico, Albuquerque, NM
- MP 130 **A small-foot print, portable 3D ion trap mass spectrometer interfaced with ambient ionization sources for the undergraduate teaching laboratory;** Caleigh R O'Connor<sup>1</sup>; Vladimir M. Doroshenko<sup>1</sup>; Nivedita Bhattacharya<sup>2</sup>; Madhuri Gupta<sup>2</sup>; Jan-Christoph Wolf<sup>3</sup>; Victor Laiko<sup>1</sup>; Enrico Davoli<sup>4</sup>; Venkat Panchagnula<sup>1</sup>; <sup>1</sup>MassTech Inc., Columbia, MD; <sup>2</sup>Barefeet Analytics Pvt. Ltd., Pune, India; <sup>3</sup>Plasmion GmbH, Augsburg, Germany; <sup>4</sup>Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy

ELEMENTAL ANALYSIS  
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- MP 131 **Analysis of Elemental Impurities in Synthetic Oligonucleotides by ICP-MS In compliance with USP <232>/<233> and ICH Q3D(R2)/Q2(R1);** Yulan Bian<sup>1</sup>; Manorama Tummala<sup>1</sup>; <sup>1</sup>Agilent Technologies, Singapore, Singapore
- MP 132 **Advancing Environmental Protection Through Real-Time Mobile, Fenceline, and Ambient Air Monitoring Solutions;** Paul Johnson<sup>1</sup>; Vaughan S. Langford<sup>2</sup>; Daniel B. Milligan<sup>2</sup>; Jihoon Lee<sup>2</sup>; Minyoung Cha<sup>2</sup>; <sup>1</sup>Syft Technologies, Anaheim, CA; <sup>2</sup>Syft Technologies, Christchurch, New Zealand
- MP 133 **Monitoring degradation of lithium-ion cells as a function of chemistry and cycling conditions via inductively coupled plasma mass spectrometry;** Jessica K Kustas<sup>1</sup>; Benjamin Juba<sup>1</sup>; Yuliya Preger<sup>1</sup>; Reed Wittman<sup>1</sup>; Jill Langendorf<sup>1</sup>; Armando Fresquez<sup>1</sup>; Babu Chalamala<sup>1</sup>; <sup>1</sup>Sandia National Laboratories, Albuquerque, NM
- MP 134 **Development of Novel Instrumentation Hyphenating Inductively Coupled Plasma Mass Spectrometry with Colinear Resonance Ionisation Spectroscopy (ICP-MS-CRIS);** Giles Edwards<sup>1</sup>; Matthew Duggan<sup>1</sup>; Holly Perrett<sup>1</sup>; Jordan Reilly<sup>1</sup>; Kieran Flanagan<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, United Kingdom
- MP 135 **Unraveling Arsenic Speciation in Varied Food Matrices: Exploring Variability in High-Arsenic Foods;** Rachel R. Jones<sup>1</sup>; Kaitlyn Maloley<sup>1</sup>; Jacqueline Michelle Chaparro<sup>1,2</sup>; Jessica E. Prenni<sup>1</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO; <sup>2</sup>Analytical Resources Core: Bioanalysis and Omics Center, Colorado State University, Fort Collins, CO

ENERGY: PETROLEUM, BIOFUELS, AND ALGAE  
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- MP 136 **Online Chemical Analysis of Flowing Hydrocarbon Fuel Surrogates in a Pyrolysis Reactor by Molecular Beam Mass Spectrometry;** Andrew DeBlase<sup>1,2</sup>; Matthew C Rohan<sup>2</sup>; Elizabeth S Kurian<sup>2</sup>; Alexander D Tucker<sup>2</sup>; Christopher R Bruening<sup>1,2</sup>; William K Lewis<sup>2</sup>; <sup>1</sup>University of Dayton Research Institute, Dayton, OH; <sup>2</sup>Air Force Research Laboratory, Aerospace Systems Directorate, Dayton, OH
- MP 137 **PETROLEUM AND ITS DISTILLATION CUTS ASSESSMENT: POLAR COMPOUNDS CHARACTERIZATION BY ORBITRAP HIGH**

**RESOLUTION MASS SPECTROMETRY;** Thamara Barra<sup>1</sup>; Dayane Magalhães Coutinho<sup>1</sup>; Gutierri Ricardo dos Santos Gonçalves Salgueiro<sup>1</sup>; Alexandre de Oliveira Gomes<sup>2</sup>; Francisco Radler De Aquino Neto<sup>1</sup>; Débora de Almeida Azevedo<sup>1</sup>; <sup>1</sup>UFRJ - Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; <sup>2</sup>PETROBRAS, Rio de Janeiro, Brazil

- MP 138 **Complementarity of on-line RPLC x SFC-qTOF and SFC-FTICR for microalgae bio-oil characterization;** Jason Devaux<sup>1,2,3</sup>; Mélanie Mignot<sup>1,3</sup>; Caroline Barrère-Mangote<sup>3,4</sup>; Pierre Giusti<sup>3,4</sup>; Sabine Heinisch<sup>2</sup>; Carlos Afonso<sup>1,3</sup>; <sup>1</sup>Laboratoire COBRA, Mont-Saint-Aignan Cedex, France; <sup>2</sup>Institut des Sciences Analytiques, Villeurbanne, France; <sup>3</sup>International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France; <sup>4</sup>TotalEnergies, Harfleur, France

- MP 139 **Characterization of re-refined base oils for lubricants using statistical approaches on Orbitrap mass spectrometry data;** Oscar Lacroix-Andrivet<sup>1,2,3</sup>; Marie Hubert-Roux<sup>3,4</sup>; Anna Luiza Mendes Siqueira<sup>2,3</sup>; Corinne Loutelier Bourhis<sup>4</sup>; Carlos Afonso<sup>3,4</sup>; <sup>1</sup>University of Rouen-Normandy, Mont-Saint-Aignan, France; <sup>2</sup>TotalEnergies OneTech, Centre de Recherche de Solaize (CRES), Chemin du canal, BP 22, 69360 Solaize, France, Solaize, France; <sup>3</sup>International Joint Laboratory—iC2MC: Complex Matrices Molecular Characterization, TRTG, BP 27, 76700 Harfleur, France, Harfleur, France; <sup>4</sup>Normandie Univ, COBRA, UMR6014 and FR3038, Université de Rouen, INSA de Rouen, CNRS, IRCOF, 1 rue Tesnière, 76821, Mont-Saint-Aignan Cedex, France, Mont-Saint-Aignan, France

- MP 140 **Brazilian crude oils compositional variations elucidated by pixel-based untargeted GCxGC-TOFMS data analysis;** Mônica Cardoso Santos<sup>1</sup>; Dayane Magalhães Coutinho<sup>1</sup>; Clarisse Lacerda Torres<sup>1</sup>; Manoel Mendes Alves Junior<sup>1</sup>; Michele Fabri de Resende<sup>1</sup>; Thamara Andrade Barra<sup>1</sup>; Vinícius Barreto Pereira<sup>1</sup>; Daniel Silva Dubois<sup>2</sup>; Joelma Pimentel Lopes<sup>2</sup>; Francisco Radler Aquino Neto<sup>1</sup>; Débora de Almeida Azevedo<sup>1</sup>; <sup>1</sup>UFRJ - Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; <sup>2</sup>PETROBRAS, Rio de Janeiro, Brazil

- MP 141 **Direct Analysis of Petroleum and Biofuels with FT-ICR MS and Direct Ionization Probe APPI;** Samuel P Putnam; Bruker Scientific, Billerica, MA

- MP 142 **Biofuel extraction by ammonia from microalgal feed stock;** Takashi Ted Nohmi<sup>1,2</sup>; Kiyoshi Sakuragi<sup>3</sup>; Toshio Mogi<sup>2</sup>; <sup>1</sup>HysafeNohmi, Setagaya-Ku, Japan; <sup>2</sup>The university of Tokyo Department of Chemical System Engineering, Tokyo, Japan; <sup>3</sup>Central Research Institute of Electric Power Industry, Yokosuka, Japan

- MP 143 **Characterization of vacuum pump oils containing complex mixtures by combining multiple MS methods;** Kirk R Jensen<sup>1</sup>; Robert B Cody<sup>1</sup>; A John Dane<sup>1</sup>; <sup>1</sup>JEOL USA, Inc., Peabody, MA

- MP 144 **Enhancing Petroleomics: Integrated Online SPE in FT-ICR MS for Complex Mixture Analysis – New solutions to Older Problems;** Nerilson MARQUES LIMA<sup>1</sup>; Hugo G Machado<sup>2</sup>; Gesiane da Silva Lima<sup>2</sup>; Jovellton Batista Da Silva Junior<sup>2</sup>; Gabriel Franco Dos Santos<sup>2</sup>; Andréa Rodrigues Chaves<sup>2</sup>; Alexandre A Ferreira<sup>3</sup>; Ygor S. Rocha<sup>3</sup>; Rodrigo Cabral da Silva<sup>3</sup>; Boniek Gontijo Vaz<sup>2</sup>; <sup>1</sup>FEDERAL UNIVERSITY OF GOIAS, Goiânia, Brazil; <sup>2</sup>Federal University of Goiás, Goiânia, Brazil; <sup>3</sup>PETROBRAS, Rio de Janeiro, Brazil

- MP 145 **Hidden Helpers: Metabolomic Analyses of Algae and Plants Reveal Dramatically Altered Metabolite Production in the Presence of Growth Promoting Bacteria;** Austin R Anderson<sup>1,2</sup>; Sangeeta Negi<sup>3</sup>; Brett R. Blackwell<sup>1,2</sup>; Kayla Kozisek<sup>4</sup>; Eric Robert Moore<sup>3</sup>; Abigale S Mikolitis<sup>1,2</sup>; Emilio S. Rivera<sup>1,2</sup>; Chi-Yen Tseng<sup>1,2</sup>; Ethan M. McBride<sup>1,2</sup>; Phillip M. Mach<sup>1,2</sup>; Zachary J. Sasiene<sup>1,2</sup>; Grace M. Thornhill<sup>1,2</sup>; Erick S. LeBrun<sup>1,2</sup>; Joshua D. Breidenbach<sup>1,2</sup>; Salvator J. Palmisano<sup>1,2</sup>; Jessica A. Salguero<sup>1,2</sup>; Francisca E. Rodriguez<sup>1,2</sup>; Tara Harvey<sup>1,2</sup>; Kes A. Luchini<sup>1,2</sup>; Trevor G.

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- Glaros<sup>1,2</sup>; Lauren K. Heine<sup>1,2</sup>; <sup>1</sup>Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>3</sup>Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>4</sup>High Explosives Science and Technology Group, Weapon Stockpile Modernization Division, Los Alamos National Laboratory, Los Alamos, New Mexico
- MP 146 **Ageing effects of renewable synthetic and fossil fuels in a simulated technical environment;** Laurin Grabler<sup>1</sup>; Alessandro Vetere<sup>1</sup>; Wolfgang Schrader<sup>1</sup>; <sup>1</sup>Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany
- MP 147 **Comparison of lignocellulosic-based biomass pyrolysis processes by multi-scale molecular characterization;** Charlotte MASE<sup>1,2</sup>; Rémi Mouliau<sup>1,2</sup>; Eliane Lazzari<sup>3</sup>; Marco Piparo<sup>1,2</sup>; Marie HUBERT-ROUX<sup>2,4</sup>; Carlos AFONSO<sup>2,4</sup>; David C. Dayton<sup>5</sup>; Caroline Barrère-Mangote<sup>1,2</sup>; Pierre Giusti<sup>1,2</sup>; <sup>1</sup>TOTALENERGIES OT, Harfleur, France; <sup>2</sup>International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France; <sup>3</sup>Organic and Biological Analytical Chemistry Group, MolSys Research Unit, Liège, Belgium; <sup>4</sup>Univ Rouen Normandie, Rouen, France; <sup>5</sup>RTI International, Technology Advancement and Commercialization, Research Triangle Park, NC
- MP 148 **How can we gain structural information about individual compounds in complex mixtures: High resolution mass spectrometry meets theoretical calculations;** Wolfgang Schrader<sup>1</sup>; Jens Dreschmann<sup>1</sup>; Zahra Farmani<sup>1</sup>; Alessandro Vetere<sup>1</sup>; <sup>1</sup>Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany
- MP 149 **Molecular characterization in Lithium-ion batteries: from electrolytes to electrodes;** Julien Maillard<sup>1,2</sup>; Julien Demeaux<sup>3</sup>; Charlotte MASE<sup>1,2,4</sup>; Antonin Gajan<sup>3</sup>; Cécile Tessier<sup>3</sup>; Patrick Bernard<sup>3</sup>; Pierre Giusti<sup>2,4,5</sup>; Carlos Afonso<sup>2,4</sup>; <sup>1</sup>TOTALENERGIES OT, Harfleur, France; <sup>2</sup>International Joint Laboratory—iC2MC: Complex Matrices Molecular Characterization, TRTG, BP 27, 76700 Harfleur, France, Harfleur, France; <sup>3</sup>SAFT, Bordeaux, France; <sup>4</sup>University of Rouen-Normandie, Mont-Saint-Aignan, France; <sup>5</sup>TotalEnergies, Harfleur, France
- MP 150 **Utilizing a novel splitter to eliminate quantitation bias for simultaneous GCxGC-TOFMS/FID characterization of traditional and emerging fuels;** David E Alonso<sup>1</sup>; Joseph E Binkley<sup>1</sup>; John Hayes<sup>1</sup>; Elizabeth M Humston-Fulmer<sup>1</sup>; Christina N Kelly<sup>1</sup>; Dave Russ<sup>1</sup>; <sup>1</sup>LECO Corporation, Saint Joseph, MI
- MP 151 **Optimization of Interfacial Material Isolation in Water-Oil Emulsions and Characterization by ESI(-)FT-ICR MS: A Centrifugation Method Approach;** Lindamara Maria de Souza<sup>1,2</sup>; Eliane Valéria de Barros<sup>3</sup>; Luciana Costa De Souza<sup>1</sup>; Gabrieli Silveira Folli<sup>1</sup>; Cristina Maria dos Santos Sad<sup>1</sup>; Danielle Mitze Muller Franco<sup>4</sup>; Gabriel Henry Morais Dufraayer<sup>4</sup>; Boniek Gontijo Vaz<sup>4</sup>; Marcio Nele de Souza<sup>5</sup>; Osvaldo Karnitz Jr<sup>6</sup>; Luiz Silvino Chinelatto Jr<sup>6</sup>; Marcia Cristina Khalil de Oliveira<sup>6</sup>; Valdemar Lacerda Jr<sup>1</sup>; Wanderson Romão<sup>2,7,8</sup>; <sup>1</sup>Federal University of Espírito Santo, Vitória, Brazil; <sup>2</sup>National Institute of Forensic Science and Technology, INCT, Porto Alegre, Brazil; <sup>3</sup>Federal Institute of Education, Science and Technology of Espírito Santo, Vitória, Brazil; <sup>4</sup>Federal University of Goiás, Goiania, Brazil; <sup>5</sup>Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; <sup>6</sup>PETROBRAS, Rio de Janeiro, Brazil; <sup>7</sup>Federal Institute of Education, Science and Technology of Espírito Santo, Vila Velha, Brazil; <sup>8</sup>Federal University of Espírito Santo, Vitória, Brazil
- MP 152 **ESI(-)FT-ICR MS applied in the study of interfacial materials of Brazilian crude oils;** Eliane Valéria de Barros<sup>1</sup>; Lindamara Maria de Souza<sup>2</sup>; Luciana Costa De Souza<sup>3</sup>; Cristina Maria dos Santos Sad<sup>3</sup>; Danielle Mitze Muller Franco<sup>4</sup>; Gabriel Henry Morais Dufraayer<sup>4</sup>; Boniek Gontijo Vaz<sup>4</sup>; Marcio Nele de Souza<sup>5</sup>; Osvaldo Karnitz Jr<sup>6</sup>; Luiz Silvino Chinelatto Jr<sup>6</sup>; Marcia Cristina Khalil de Oliveira<sup>6</sup>; Valdemar Lacerda Jr<sup>1</sup>; Wanderson Romão<sup>2,7,8</sup>; <sup>1</sup>Federal University of Espírito Santo, Vitória, Brazil; <sup>2</sup>National Institute of Forensic Science and Technology, INCT, Porto Alegre, Brazil; <sup>3</sup>Federal Institute of Education, Science and Technology of Espírito Santo, Vitória, Brazil; <sup>4</sup>Federal University of Goiás, Goiania, Brazil; <sup>5</sup>Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; <sup>6</sup>PETROBRAS, Rio de Janeiro, Brazil; <sup>7</sup>Federal Institute of Education, Science and Technology of Espírito Santo, Vila Velha, Brazil; <sup>8</sup>Federal University of Espírito Santo, Vitória, Brazil
- MP 153 **Direct APCI: A Straightforward Method for Precision Analysis of Sulfur-Containing Compounds in Complex Mixtures;** Danielle Mitze<sup>1</sup>; Taynara Covas<sup>1</sup>; Rosana Cardoso<sup>1</sup>; Lidya Cardozo<sup>1</sup>; Mário Rangel<sup>1</sup>; Rosineide Simas<sup>2</sup>; Gabriel Henry Dufraayer<sup>1</sup>; Boniek Gontijo<sup>1</sup>; <sup>1</sup>Federal University of Goiás, Goiania, Brazil; <sup>2</sup>Mackenzie University, São Paulo, Brazil
- MP 154 **Finding needles in haystacks: Using statistical tools for complex samples measured by using GCxGC-HRMS;** John Dane<sup>1</sup>; Scott J. Campbell<sup>2</sup>; John Moncur<sup>2</sup>; Kirk R Jensen<sup>1</sup>; Robert B Cody<sup>1</sup>; <sup>1</sup>JEOL USA, Inc., Peabody, MA; <sup>2</sup>SpectralWorks Ltd, Runcorn, United Kingdom
- MP 155 **Influence of Metals On Asphaltenes' ESR, Ion Mobility, Mass, and NMR Spectra: An Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) Study;** Sahil Makhani<sup>1</sup>; Thanuja M Thilakarathna<sup>1</sup>; Bismark Nyaabak<sup>1</sup>; Patrick J. Farmer<sup>1</sup>; Touradj Solouki<sup>1</sup>; <sup>1</sup>Baylor University, Waco, TX

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- MP 156 **Measurement of Medium and Long Chlorinated Alkanes in Canadian Biota and Analysis by LC Orbitrap;** Helena Steer<sup>1</sup>; Beau Atkinson<sup>1</sup>; Adnan Chowdhury<sup>1,2</sup>; <sup>1</sup>Environment Canada, Burlington, ON; <sup>2</sup>Western University, London, ON
- MP 157 **A Penguin's Perspective: Silicone wristbands as passive samplers to explore exposure of Megellanic Penguins to emerging and legacy contaminants;** Paige Montgomery<sup>1</sup>; Jonathan Navarro-Ramos<sup>1</sup>; Ralph Eric Thijl Vanstreels<sup>2</sup>; Logan Running<sup>1</sup>; Katarzyna Kordas<sup>3</sup>; Diana S Aga<sup>1,4</sup>; <sup>1</sup>Department of Chemistry, The State University of New York at Buffalo, Buffalo, NY; <sup>2</sup>University of São Paulo. Department of Pathology, Laboratory of Comparative Pathology of Wild Animals, Butantã, Brazil; <sup>3</sup>Department of Epidemiology and Environmental Health, The State University of New York at Buffalo, Buffalo, NY; <sup>4</sup>RENEW Institute, The State University of New York at Buffalo, Buffalo, NY
- MP 158 **Non-target Identification of Harmful Organic Compounds in Weathered Marine Microplastics by High-Resolution Gas Chromatography-Time-of-Flight-Mass Spectrometry;** Patrick T Justen<sup>1</sup>; Emily Böckenholt<sup>2</sup>; Susan D Richardson<sup>1</sup>; Mohammed Baalousha<sup>1</sup>; <sup>1</sup>University of South Carolina, Columbia, SC; <sup>2</sup>University of Duisburg Essen, Duisburg, Germany
- MP 159 **Characterizing novel, sorbent-based pre-concentration methods for trace detection of perfluoroalkyl substances with ambient pressure mass spectrometry;** Nathan Robert Bays<sup>1</sup>; David Shafer<sup>1</sup>; Andre Benally<sup>1</sup>; Mohammad Shohel<sup>1</sup>; Troy Benceo<sup>1</sup>; Mark Rigali<sup>1</sup>; Jessica Kustas<sup>1</sup>; Andrew W. Knight<sup>1</sup>; Ryan D. Davis<sup>1</sup>; <sup>1</sup>Sandia National Lab, Albuquerque, NM
- MP 160 **Innovation Development of Multidimensional Holographic Analysis Technology of the Pre- and Polyfluoroalkyl Substances in Environmental Water;** Shan-An Chan<sup>1</sup>; Yue Song<sup>2</sup>; Hui XU<sup>2</sup>; <sup>1</sup>Agilent Technology, Inc., Taipei, Taiwan; <sup>2</sup>Agilent Technology, Inc., Shanghai, China
- MP 161 **Utilizing cost effective helium saving technology for low level quantitation of Polychlorinated dibenzo-p-dioxins/furans using gas chromatograph mass**

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- spectrometry; Adam Ladak<sup>1</sup>; Paul Silcock<sup>1</sup>; Nicholas Warner<sup>2</sup>; Daniel Kutscher<sup>2</sup>; Amit Gujar<sup>3</sup>; Jason Cole<sup>3</sup>; Xin Zheng<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific, Bannockburn, IL
- MP 162 **Paper Spray High-Resolution Tandem Mass Spectrometry (PS-HRMS/MS) for Rapid, Multi-class Cyanotoxin Analysis;** Lucas R. Abruzzi<sup>1, 2</sup>; Daniel G. Beach<sup>3</sup>; Erik T Krogh<sup>1, 2</sup>; Christopher G. Gill<sup>1, 2, 4, 5, 6</sup>; <sup>1</sup>Appl. Env. Res. Labs. (AERL), Nanaimo, BC; <sup>2</sup>University of Victoria, Victoria, BC; <sup>3</sup>National Research Council Canada, Halifax, NS; <sup>4</sup>Vancouver Island University, Nanaimo, BC; <sup>5</sup>Simon Fraser University, Burnaby, BC; <sup>6</sup>University of Washington, Seattle, WA
- MP 163 **Rapid and highly sensitive quantitation of Microcystins and Nodularin in water by modern LC-MS/MS;** Kate (Xiaomeng) Xia<sup>1</sup>; Evelyn Wang<sup>1</sup>; Ruth Marfil-Vega<sup>1</sup>; Yoshiyuki Okamura<sup>1</sup>; Tairo Ogura<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD
- MP 164 **Pyrolysis gas chromatography-cyclic ion mobility mass spectrometry reveals micro-/nanoplastics in placental tissue of Canadians;** Nikita E. Harvey<sup>1</sup>; Justine R. Bissonnette<sup>1</sup>; Darcie Stapleton<sup>1</sup>; Catherine M.E. Barrett<sup>1</sup>; Lindsay S. Cahill<sup>1</sup>; Karl J. Jobst<sup>1</sup>; <sup>1</sup>Memorial University of Newfoundland, St. John's, NL
- MP 165 **Characterization of microplastics in the maternal blood of Canadians by pyrolysis gas chromatography-cyclic ion mobility mass spectrometry;** Justine R. Bissonnette<sup>1</sup>; Nikita E. Harvey<sup>1</sup>; Lindsay S. Cahill<sup>1</sup>; Karl J. Jobst<sup>1</sup>; <sup>1</sup>Memorial University of Newfoundland, St. John's, NL
- MP 166 **Per- and Polyfluoroalkyl Substances in Aqueous Samples: Performance Demonstration of EPA Method 1633 Using High Sensitivity Mass Spectrometry;** Megan P. Davis<sup>1</sup>; Om K Shrestha<sup>1</sup>; Kathleen K Luo<sup>1</sup>; Landon A Wiest<sup>1</sup>; Evelyn H Wang<sup>1</sup>; Michelle Zipse<sup>1</sup>; Keith Herman<sup>1</sup>; <sup>1</sup>SSI, Columbia, MD
- MP 167 **Intensive temporal sampling for the emerging salmon toxin 6PPD quinone by condensed phase membrane introduction mass spectrometry;** Angelina Jaeger<sup>1, 2</sup>; Joseph Monaghan<sup>1</sup>; Haley Tomlin<sup>3</sup>; Jamieson Atkinson<sup>3</sup>; Chris G Gill<sup>1, 2, 4, 5</sup>; Erik T Krogh<sup>1, 2</sup>; <sup>1</sup>Vancouver Island University, Nanaimo, BC; <sup>2</sup>University of Victoria, Victoria, BC; <sup>3</sup>British Columbia Conservation Foundation, Nanaimo, BC; <sup>4</sup>Simon Fraser University, Burnaby, BC; <sup>5</sup>University of Washington, Seattle, WA
- MP 168 **Crowdsourcing Citizens for Statewide Mapping of PFAS in Florida Drinking Water;** Thomas Sinkway; University of Florida, Gainesville, FL
- MP 169 **Evaluation of Extremophile Methylorubrum extorquens for Treatment of Oilsands-Derived Naphthenic Acid Fraction Compounds by Orbitrap Mass Spectrometry;** Ian J Vander Meulen<sup>1, 2</sup>; Jordyn Bergsveinson<sup>2</sup>; Dena W McMartin<sup>1, 3</sup>; John Headley<sup>2</sup>; <sup>1</sup>University of Saskatchewan, Saskatoon, SK; <sup>2</sup>Environment Canada, Saskatoon, SK; <sup>3</sup>University of Lethbridge, Lethbridge, AB
- MP 170 **A high-throughput analysis workflow to characterize Pharmaceuticals and personal care products (PPCPs) in aquatic environment;** SHENGLAN JIA<sup>1</sup>; Mauricius Marques Dos Santos<sup>1</sup>; Shane Allen Snyder<sup>1</sup>; <sup>1</sup>Nanyang Technological University, NEWRI, Singapore, Singapore
- MP 171 **Expanding the chemical space of the fragmentation spectra-based exposure prediction model;** Helen Sepman<sup>1, 2</sup>; Drew Szabo<sup>1</sup>; Gordian Sandberg<sup>1</sup>; Ida Rahu<sup>1</sup>; Irene Pulido Campillo<sup>1</sup>; Emma Apelgren<sup>1</sup>; Anneli Kruve<sup>1, 2</sup>; <sup>1</sup>Department of Materials and Environmental Chemistry, Stockholm University, Stockholm, Sweden; <sup>2</sup>Department of Environmental Science, Stockholm University, Stockholm, Sweden
- MP 172 **Disinfection By-products from Water Chlorination Reconfirmed by Electrochemistry-MS;** Jean-Pierre Chervet<sup>1</sup>; Albert T LEBEDEV<sup>2</sup>; Martin Eysberg<sup>3</sup>; Hendrik-Jan Brouwer<sup>4</sup>; <sup>1</sup>Antec Scientific, Alphen a/d Rijn, Netherlands;
- <sup>2</sup>Department of Materials Science, MSU-BIT University, Shenzhen 517182, China; <sup>3</sup>Antec Scientific, Boston, MA; <sup>4</sup>Antec Scientific, Alphen aan den Rijn, Netherlands
- MP 173 **A novel approach for monitoring multi-classes of POPs in a single run by GC-Ion Mobility-HRMS;** Arnd Ingendoh<sup>1</sup>; Carsten Baessmann<sup>1</sup>; Javier Lopez<sup>1</sup>; Miguel Angel Perez<sup>1</sup>; Hugo Muller<sup>2</sup>; Gauthier Eppe<sup>3</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; <sup>2</sup>Mass Spectrometry Laboratory, MolSys Research Unit, Chemistry Department, University of Liège, Liege, Belgium; <sup>3</sup>Mass Spectrometry Laboratory, MolSys Research Unit, University of Liege, Liege, Belgium
- MP 174 **Sewage Proteomics: What can we learn?;** Ester Sánchez-Jiménez<sup>1, 2</sup>; Carlos Pérez-López<sup>2</sup>; Antonio Ginebreda<sup>2</sup>; Joaquin Abian<sup>1</sup>; Damià Barceló<sup>2</sup>; Montserrat Carrascal<sup>1</sup>; <sup>1</sup>Biological and Environmental Proteomics, Institute of Biomedical Research of Barcelona, Spanish National Research Council (IIBB-CSIC), Barcelona, Spain; <sup>2</sup>Water and Soil Quality Research Group, Department of Environmental Chemistry, Institute of Environmental Assessment and Water Research - Spanish National Research Council (IDAEA-CSIC), Barcelona, Spain
- MP 175 **Optimized gas chromatography-electron impact ionization-tandem mass spectrometry for simultaneous quantification of 12 novel brominated flame retardants in agricultural products;** Juyoun Lee<sup>1</sup>; Minki Shim<sup>1</sup>; Hoyjeong Lee<sup>1</sup>; Dong-Kyu Lee<sup>1</sup>; <sup>1</sup>College of Pharmacy, Chung-Ang University, Seoul, South Korea
- MP 176 **Determination of Glyphosate, Aminomethylphosphonic Acid (AMPA), and Glufosinate in Drinking Water Using Direct Analysis by LC-MS/MS;** Narendra Meruva<sup>1</sup>; Stuart J Adams<sup>2</sup>; Benjamin Wuyts<sup>3</sup>; Simon Hird<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, Massachusetts; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>3</sup>Waters Corporation, Antwerp, Belgium
- MP 177 **Expanding a High-Quality Environmental Reference Electron Ionization Mass Spectral Library;** Yufang Zheng<sup>1</sup>; Edward P. Erisman<sup>1</sup>; Weihua Ji<sup>1</sup>; Tytus Mak<sup>1</sup>; Quan-Long Pu<sup>1</sup>; Stephen E Stein<sup>1</sup>; William E Wallace<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD
- MP 178 **Harnessing the Power of Mass Spectrometry and Automation to Reduce Sample Size, Sample Preparation Time and Increase Laboratory Efficiency;** Kari Organtini<sup>1</sup>; Chelsea Plummer<sup>1</sup>; Kenneth Rosnack<sup>1</sup>; Oliver Burt<sup>2</sup>; Ian Wan<sup>3</sup>; <sup>1</sup>Waters Corporation, Milford, Massachusetts; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>3</sup>PromoChrom Technologies, Richmond, BC
- MP 179 **Analysis of High Mass Polycyclic Aromatic Hydrocarbons (PAHs) Extracted from Microplastics Spilled in the Marine Environment;** Douglas Stevens<sup>1</sup>; Christopher Reddy<sup>2</sup>; Bryan James<sup>2</sup>; Robert Nelson<sup>2</sup>; Frank L. Dorman<sup>1</sup>; Sarah Dowd<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, Massachusetts; <sup>2</sup>Woods Hole Oceanographic Institution, Falmouth, MA
- MP 180 **Suspect and non-targeted screening of halogenated contaminants in a stranded killer whale (Orcinus orca) using GC-HRMS hyphenated with TMS;** Hugo Muller<sup>1</sup>; Krishna Das<sup>2</sup>; George Scholl<sup>1</sup>; Emma L. Schymanski<sup>3</sup>; Gauthier Eppe<sup>1</sup>; <sup>1</sup>Mass Spectrometry Laboratory, MolSys Research Unit, University of Liege, Liege, Belgium; <sup>2</sup>Freshwater and Oceanic Sciences Unit of ReSearch (FOCUS), Laboratory of Oceanology, University of Liège, Liège, Belgium; <sup>3</sup>Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Luxembourg, Luxembourg
- MP 181 **Quantification of Microplastics and Nanoplastics in biosolids;** Tommy M Nguyen<sup>1</sup>; O. David Sparkman<sup>2</sup>; Liang Xue<sup>2</sup>; Harry Allen<sup>3</sup>; Terry Ramus<sup>4</sup>; Ichi Watanabe<sup>5</sup>; <sup>1</sup>University of The Pacific, Stockton, CA; <sup>2</sup>University of the Pacific, Stockton, CA; <sup>3</sup>U.S. Environmental Protection Agency, Arcadia, CA; <sup>4</sup>Diablo Analytical, Antioch, CA; <sup>5</sup>Frontier Laboratories, Koriyama, Japan

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- MP 182 **Statewide surveillance and mapping of PFAS in Florida surface water**; Camden Camacho<sup>1</sup>; John Bowden<sup>1</sup>; <sup>1</sup>University of Florida, Chemistry Department, Analytical Chemistry Division, Gainesville, FL
- MP 183 **Non-targeted analysis of complex environmental samples using thermal desorption, multi-mode ionization methods, multidimensional gas chromatography, and high-resolution mass spectrometry**; David E Alonso<sup>1</sup>; Joe Binkley<sup>2</sup>; <sup>1</sup>Leeco Corporation, St. Joseph, MI; <sup>2</sup>LECO Corporation, Saint Joseph, MI
- MP 184 **Residential exposure to micro-/nanoplastics in indoor air studied by pyrolysis gas chromatography-cyclic ion mobility mass spectrometry**; Mikela L Rowsell<sup>1</sup>; Frank L. Dorman<sup>2</sup>; Lindsay S. Cahill<sup>3</sup>; Karl J Jobst<sup>3</sup>; <sup>1</sup>Memorial University of Newfoundland, St. John's, NL; <sup>2</sup>Waters Corporation, Milford, Massachusetts; <sup>3</sup>Memorial University of Newfoundland, St. John's, NL
- MP 185 **Characterization of hydrothermal liquefaction products of kraft lignin using high-resolution ESI/APPI FT-ICR MS**; Mahmoud Negm<sup>1</sup>; Eemeli Eronen<sup>1</sup>; Mikko Nikunen<sup>1</sup>; Janne Jänis<sup>1</sup>; <sup>1</sup>University of Eastern Finland, Joensuu, Finland
- MP 186 **Effect of ionic strength on adsorption of microcystins and nodularin-R onto corncob-based activated carbon and optimization of batch adsorption parameters**; Hasaruwani S Kiridena<sup>1</sup>; Michal Marszewski<sup>1</sup>; Dragan Isailovic<sup>1</sup>; <sup>1</sup>University of Toledo, Toledo, OH
- MP 187 **Identification of Novel Cyanopeptolins in Lake Erie CyanoHAB Samples using UHPLC-HRMS and HRMS/MS**; Sharmila I Thenuwara<sup>1</sup>; Judy A Westrick<sup>2</sup>; Dragan Isailovic<sup>1</sup>; <sup>1</sup>University of Toledo, Toledo, OH; <sup>2</sup>Wayne State University, Detroit, MI
- MP 188 **Identification of Degradation Products of Cellulose Derivatives in Soil**; Cole D. Babcock<sup>1,2</sup>; Ayden S Justice-Riar<sup>1</sup>; Seth Nobert<sup>1</sup>; Emmanuel Mapfumo<sup>1</sup>; Makan Golizeh<sup>1</sup>; <sup>1</sup>Concordia University of Edmonton, Edmonton, AB; <sup>2</sup>Babcocks Synthetics Ltd., Wainwright, AB
- MP 189 **Rapid Degradation of Per- and Polyfluoroalkyl Substances (PFAS) in Microdroplets**; Md. Tanim-Al Hassan<sup>1</sup>; Yongqing Yang<sup>1</sup>; Richard N Zare<sup>2</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>New Jersey Institute of Technology, Newark, NJ; <sup>2</sup>Stanford University, Stanford, CA
- MP 190 **Improved cyanobacterial harmful algal bloom toxin panel using liquid chromatography with triple quadrupole mass spectrometry and orbitrap mass spectrometry**; Dwayne E Schrunk; 1515B College of Veterinary Medicine, Ames, IA
- MP 191 **Soot-on-snow: Comprehensive chemical fingerprinting of combustion-derived organic aerosols deposited on snow using APPI/ESI FT-ICR mass spectrometry**; Timo Kekäläinen<sup>1</sup>; Mikko Nikunen<sup>1</sup>; Hans Moosmüller<sup>2</sup>; Jonas Svensson<sup>3</sup>; Krista Luoma<sup>3</sup>; Delun Li<sup>3</sup>; Outi Meinander<sup>3</sup>; Anna Kontu<sup>4</sup>; Oona Norvapalo<sup>5</sup>; Pavla Dagsson-Waldhauserova<sup>6</sup>; Aki Virkkula<sup>3</sup>; Olli Sippula<sup>5</sup>; Janne Jänis<sup>1</sup>; Jie Guo<sup>1</sup>; Niko Kinnunen<sup>1</sup>; <sup>1</sup>University of Eastern Finland, Joensuu, Finland; <sup>2</sup>Division of Atmospheric Sciences, Desert Research Institute (DRI), Reno, NV; <sup>3</sup>Atmospheric Composition Unit, Finnish Meteorological Institute, Helsinki, Finland; <sup>4</sup>Earth Observation Research, Finnish Meteorological Institute, Sodankylä, Finland; <sup>5</sup>Department of Environmental and Biological Sciences, University of Eastern Finland, Kuopio, Finland; <sup>6</sup>Faculty of Environmental and Forest Sciences, Agricultural University of Iceland, Reykjavik, Iceland
- MP 192 **Method Development and Validation for Trace Determination of Aryl and Alkyl Organophosphate Esters in Surface Waters by LC-MSMS**; Beau W Atkinson<sup>1</sup>; JoAnne Schachtschneider<sup>1</sup>; <sup>1</sup>Environment Canada, Burlington, ON
- MP 193 **Determination of emerging contaminants in ambient water using an ultra-sensitive triple quadrupole mass spectrometer**; Guangning Li<sup>1</sup>; Xiaojie Sun<sup>2</sup>; Bingjie Liu<sup>2</sup>; Lihai Guo<sup>2</sup>; <sup>1</sup>SCIEX, Beijing, China; <sup>2</sup>SCIEX, Beijing, China
- MP 194 **Evaluation of Dielectric Barrier Discharge Ionization (DBDI) for the Identification of Xenobiotic Environmental Metabolites and Degradation Products**; Jeffrey R Gilbert<sup>1</sup>; David K Robbins<sup>1</sup>; Chris Brown<sup>1</sup>; Krishna Kuppanan<sup>1</sup>; David Hills<sup>1</sup>; Chengli Zu<sup>1</sup>; <sup>1</sup>Corteva Agriscience, Indianapolis, IN
- MP 195 **LC-MS/MS assay for Quantitative Analysis of Long Acting Anti Coagulants (LAARs) in Plasma and Extracellular Vesicles from Rabbits**; Intakhar Ahmad<sup>1</sup>; Ruth N Muchiri<sup>2</sup>; Richard B van Breemen<sup>2</sup>; Douglas Feinstein<sup>1</sup>; <sup>1</sup>University of Illinois at Chicago, Chicago, IL; <sup>2</sup>Oregon State University, Corvallis, OR
- MP 196 **Assessing Antidepressant Pharmaceuticals in the Environment through the Development of a Multidimensional Liquid Chromatography-Ion Mobility Spectrometry-Mass Spectrometry Library**; Emily K Crawford<sup>1</sup>; James N. Dodds<sup>1</sup>; Erin S. Baker<sup>1</sup>; <sup>1</sup>UNC-Chapel Hill, Chapel Hill, NC
- MP 197 **Characterization of organic and inorganic analytes in snow made from reclaimed water at Arizona Snowbowl Ski Resort**; Marquis T. Yazzie<sup>1</sup>; Haoqi Nina Zhao<sup>2</sup>; Anita J. Antoninka<sup>3</sup>; Pieter C. Dorrestein<sup>2</sup>; Catherine R. Propper<sup>3</sup>; Jani C. Ingram<sup>3</sup>; Allegra T. Aron<sup>1</sup>; <sup>1</sup>University of Denver, Denver, CO; <sup>2</sup>University of California San Diego, La Jolla, CA; <sup>3</sup>Northern Arizona University, Flagstaff, AZ
- MP 198 **Format Comparison for Dispersive Solid Phase Extraction (dSPE) Workflow Improvements for Food Testing Prior to GC/MS Analysis**; Lucy Lund<sup>1</sup>; Russell Parry<sup>1</sup>; Lee Williams<sup>1</sup>; Geoff Davies<sup>1</sup>; Alan Edgington<sup>1</sup>; Adam Senior<sup>1</sup>; Helen Lodder<sup>1</sup>; Zainab Khan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Dan Menasco<sup>1</sup>; <sup>1</sup>Biotage GB Limited, Cardiff, United Kingdom
- MP 199 **Comprehensive pesticide screening by column-switching LC-MS/MS using multiple activation methods CID, EAD and UVPD**; Romain GIRAUD<sup>1</sup>; Mircea Guna<sup>2</sup>; Yves LeBlanc<sup>2</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>LSMS, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; <sup>2</sup>SCIEX, Concord, ON
- MP 200 **Making Crayfish Happy: Using LC-MS/MS to Evaluate the Nervous System of Procambarus clarkii Following Exposure to SSRIs and SNRIs**; Claire Korte<sup>1</sup>; Sydney Worth<sup>1</sup>; Jillian Tonnies<sup>1</sup>; Corina Trapp<sup>1</sup>; Muskan Bakshi<sup>1</sup>; Kevin Tucker<sup>1</sup>; <sup>1</sup>Southern Illinois University Edwardsville, Edwardsville, IL
- MP 201 **Extractive-Liquid Sampling Electron Ionization-Mass Spectrometry (E-LEI-MS) for real-time targeted and non-targeted analysis of pesticides and active pharmaceutical ingredients**; Adriana Arigo<sup>1</sup>; Giovanna Nevola<sup>1</sup>; Giorgio Famigliani<sup>1</sup>; Pierangela Palma<sup>1,2</sup>; Achille Cappiello<sup>1,2</sup>; <sup>1</sup>University of Urbino Carlo Bo, Urbino, Italy; <sup>2</sup>Vancouver Island University, Nanaimo, BC
- MP 202 **MALDI MSI Matrix Optimization for the Analysis of Lipid-Related Metabolites in Earthworms Exposed to Statins as Environmental Contaminants**; Kendra G. Selby<sup>1</sup>; Lauren H. Phan<sup>1</sup>; Claire E. Korte<sup>1</sup>; Gabriel A. Bressendorff<sup>1</sup>; M Nazim Boutaghou<sup>2</sup>; Kevin R. Tucker<sup>1</sup>; <sup>1</sup>Southern Illinois University Edwardsville, Edwardsville, IL; <sup>2</sup>Shimadzu Scientific Instruments, Columbia, MD
- MP 203 **Identification of anthropogenic compounds in stream waters using non-target strategies by HRMS**; Imma Ferrer<sup>1</sup>; Michael Thurman<sup>1</sup>; James S Pyke<sup>2</sup>; Andrew McEachran<sup>2</sup>; <sup>1</sup>University of Colorado, Boulder, CO; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- MP 204 **Non-Target HRMS: Quantifying Emerging Contaminants in Saudi Arabian Water, Soil, and Plants under Extreme Climate (40-45°C)**; Damia Barcelo<sup>1</sup>; Yolanda Pico<sup>2</sup>; Julian Campo<sup>2</sup>; Mohamed El-Sheik<sup>3</sup>; Ahmed H Alfarhan<sup>3</sup>; <sup>1</sup>IDAEA-CSIC, Barcelona, Spain; <sup>2</sup>SAMA-UV, Moncada, Spain; <sup>3</sup>King Saud University, Riyadh, Saudi Arabia
- MP 205 **Ultra-Sensitive Dynamic Headspace GC-MS/MS method for trace level quantitation of Nitrosamines in Deferiprone API**; Durvish Sawant<sup>1</sup>; Hemant Kesarkar<sup>1</sup>

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- Sanket Chiplunkar<sup>1</sup>; Prashant Hase<sup>1</sup>; Aseem Wagle<sup>1</sup>; Rahul Dwivedi<sup>1</sup>; Siddhata Jadhav<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; Pratap Rasam<sup>1</sup>; Satyendra Singh<sup>1</sup>; Mohit Sharma<sup>1</sup>; <sup>1</sup>*Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*
- MP 206 **Simultaneous determination of known and unknown Extractables in pharmaceuticals packaging material by tandem mass spectrometry using Scan-MRM mode; Hemant Kesarkar<sup>1</sup>; Sanket Chiplunkar<sup>1</sup>; Prashant Hase<sup>1</sup>; Durvesh Sawant<sup>1</sup>; Aseem Wagle<sup>1</sup>; Rahul Dwivedi<sup>1</sup>; Siddhata Jadhav<sup>1</sup>; Satyendra Singh<sup>1</sup>; Mohit Sharma<sup>1</sup>; Pratap Rasam<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; <sup>1</sup>*Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India***

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- MP 207 **Enhanced Detection Sensitivity of Volatile Extractables in Aqueous Extracts through Dynamic Headspace GC-MS Analysis; Samantha I Wickramasekara<sup>1</sup>; Milani Wijeweera Patabandige<sup>1</sup>; Amali Herath<sup>1</sup>; Jacob Hill<sup>1</sup>; <sup>1</sup>*U.S. Food and Drug Administration, Silver Spring, MD***
- MP 208 **GC/MS approach for analysis of extractables and leachables (E&L) in complex matrices using spectral deconvolution and retention indices; Bruce Kimby<sup>1</sup>; Anastasia Andrianova<sup>1</sup>; Sofia Nieto<sup>1</sup>; Lakshmi Krishnan<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Wilmington, DE*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA***
- MP 209 **Combined qualitative and quantitative analysis of food packaging materials using QTOF mass spectrometry; Jack Steed<sup>1</sup>; Jianru Stahl-Zeng<sup>2</sup>; Daqiang Pan<sup>2</sup>; Clemens Bidmon<sup>3</sup>; <sup>1</sup>*SCIEX, Macclesfield, United Kingdom*; <sup>2</sup>*SCIEX, Darmstadt, Germany*; <sup>3</sup>*TÜV Rheinland, Nuremberg, Germany***
- MP 210 **Combined LC/MS and GC/MS approach for analysis of extractables and leachables in complex matrices using high resolution mass spectrometry; Sofia Nieto<sup>1</sup>; David Weil<sup>1</sup>; Matthew Curtis<sup>1</sup>; Lee Bertram<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Inc., Santa Clara, CA***
- MP 211 **Effects of Extraction Conditions and Sample Preparation on Extractables from Medical Devices by LC-UV/MS; JoAnn C Chen<sup>1</sup>; Peifeng Hu<sup>1</sup>; D. Paul Cole<sup>1</sup>; <sup>1</sup>*Baxter Healthcare Corporation, Round Lake, IL***
- MP 212 **Identification and Profiling of an Unknown in Base E-Liquid Formulations; Diane Wallace<sup>1</sup>; Aliya Al-Habsha<sup>1</sup>; Matthew Lyndon<sup>1</sup>; Xin Yang<sup>1</sup>; Karen Carter<sup>1</sup>; Norman Fraley<sup>1</sup>; I. Gene Gillman<sup>1</sup>; <sup>1</sup>*Juul Labs, Washington, DC***
- MP 213 **Employing Novel Sample Preparation and Analysis by GC-TOFMS for Improved Target and Non-target Detection of Leachables in Cream/Gel Drug Products; Joseph E Binkley<sup>1</sup>; Eric Hill<sup>2</sup>; <sup>1</sup>*LECO Corporation, St. Joseph, MI*; <sup>2</sup>*Boston Analytical, Salem, NH***
- MP 214 **Headspace-SIFT-MS: Rapid Screening of Hazardous Volatile Impurities in Haircare and Skincare Products; Luke Thomason<sup>1</sup>; Mark J. Perkins<sup>2</sup>; Colin J. Hastie<sup>2</sup>; Vaughan S. Langford<sup>1</sup>; Leslie P. Silva<sup>3</sup>; <sup>1</sup>*Syft Technologies, Christchurch, New Zealand*; <sup>2</sup>*Element Lab Solutions, Cambridge, United Kingdom*; <sup>3</sup>*Syft Technologies, Los Angeles, CA***
- MP 215 **Determination of Multiple Compounds of Interest in Highly Complex Samples using GC-MS and LC-MS; Challenges in Extractables and Leachables Analysis; Michael S. Young<sup>1</sup>; Becky Bader<sup>1</sup>; Norma Turner<sup>1</sup>; <sup>1</sup>*Cambridge Polymer Group, Woburn, MA***
- MP 216 **Non-targeted analysis, interactive visualization, and online sharing of interactive LC-HRMS/MS data of polymers using a comprehensive software PolyMatch Suite; Jeremy Koelmel<sup>1</sup>; David A Weil<sup>2</sup>; Emma E. Rennie<sup>2</sup>; Paul Stelben<sup>1</sup>; Nicholas Oranzi<sup>3</sup>; Michael Kummer<sup>4</sup>; David Godri<sup>5</sup>; Jiarong Qi<sup>1</sup>; Elizabeth Z. Lin<sup>1</sup>; Krystal J. Godri Pollitt<sup>1</sup>; <sup>1</sup>*Yale University, New Haven, CT*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*; <sup>3</sup>*University of Florida, Gainesville, FL*; <sup>4</sup>*Innovative Omics, Sarasota, FL*; <sup>5</sup>*3rd Floor Solutions, Caledon, Ontario***

- MP 217 **Comparative Study of High-Resolution Q-TOF Fast Polarity Switching versus Single Polarity Data Acquisition on Mass Accuracy, Resolution and Analytical Sensitivity; David A Weil<sup>1</sup>; Lee Bertram<sup>1</sup>; Sierra D. Durham<sup>1</sup>; Olivier Chevallier<sup>1</sup>; Kai Chen<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Santa Clara, CA***

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- MP 219 **Metabolomic and Proteomic Analysis Reveals Compositional Differences in Beer Clarified Using Ultrasonic Filtration as Compared to Centrifugation; Brett R Blackwell<sup>1</sup>; James E Coons<sup>2</sup>; Chi-Yen Tseng<sup>1</sup>; Kes A. Luchini<sup>1</sup>; Bert Boyce<sup>3</sup>; Jeff Erway<sup>4</sup>; Joel Gregory<sup>5</sup>; Rich Headley<sup>6</sup>; Phillip M. Mach<sup>1</sup>; Trevor G. Glaros<sup>1</sup>; <sup>1</sup>*Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM*; <sup>2</sup>*Los Alamos National Laboratory, Los Alamos, NM*; <sup>3</sup>*Santa Fe Brewing Company, Santa Fe, NM*; <sup>4</sup>*La Cumbre Crewing Company, Albuquerque, NM*; <sup>5</sup>*Ex Novo Brewing Company, Corrales, NM*; <sup>6</sup>*Beer Creek Brewing Company, Santa Fe, NM***
- MP 220 **Identification of Double-Bond Position in Cyclic Ester using OAD-TOF system; Yohei Arai<sup>1</sup>; Jun Kurabe<sup>2</sup>; Hidenori Takahashi<sup>1</sup>; Akihiro Kawaraya<sup>2</sup>; <sup>1</sup>*Shimadzu Corporation, Nakagyo-ku, Japan*; <sup>2</sup>*TAKASAGO INTERNATIONAL CORPORATION, Hiratsuka, Japan***
- MP 221 **Characterization of Dietary Xylans and Arabinoxylans by LC-MS: Implications for Enhancement of Prebiotic Activity with Supplemental Enzymes In Situ; James G Farnar<sup>1</sup>; Caroline H. Best<sup>1</sup>; Kelly M. Tinker<sup>1</sup>; Sean M. Garvey<sup>1</sup>; <sup>1</sup>*BIO-CAT, Troy, VA***
- MP 222 **Non-targeted analysis of mushroom-containing coffee products using ion mobility-high resolution mass spectrometry; Lindsay E Hatch<sup>1</sup>; Gordon T Fujimoto<sup>1</sup>; Emily R Britton<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA***
- MP 223 **Pair derivatization Strategy using DMAQ-12C/14N and DMAQ-13C/15N for Highly Sensitive and Accurate analysis of fatty acids by LC-MS; QINGSHI MENG<sup>1</sup>; Zhenghua Rao<sup>2</sup>; Yaxiong Jia<sup>3</sup>; <sup>1</sup>*Institute of Animal Sciences, CAAS, Beijing, China*; <sup>2</sup>*Institute of Animal Sciences of Chinese Academy of Agricultural Sciences, BEIJING, China*; <sup>3</sup>*Institute of Animal Sciences, Chinese Academy of Agricultural Sciences, BEIJING, China***
- MP 224 **Discovery of Synthetic Cooling Agents in Consumer Products using a Standardized Screening Approach; Benjamin Katz; *UC Irvine, Irvine***
- MP 225 **Comprehensive Metabolomic Profiling of Coffea canephora Coffees during roasting stages by ESI(±)LTQ MS; Eustaquio V. R. De Castro<sup>1, 2</sup>; Danieli G. Debona<sup>1</sup>; Marcos Valério V. Lyrio<sup>1, 3</sup>; Lucas L. Pereira<sup>4</sup>; Amanda E. Feu<sup>3</sup>; Emanuele C. S. Oliveira<sup>4</sup>; Roberta Q. Frinhan<sup>1</sup>; Wanderson Romao<sup>3, 5</sup>; <sup>1</sup>*Coffee Chemistry Laboratory - Coffee Design Group, Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil*; <sup>2</sup>*Laboratory for Research and Development of Methodologies for Oil Analysis / LabPetro, Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil*; <sup>3</sup>*Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil*; <sup>4</sup>*Coffee Design. Federal Institute of Espírito Santo, Venda Nova do Imigrante, Brazil*; <sup>5</sup>*Federal Institute of Espírito Santo, Brazil, Vitoria, Brazil***
- MP 226 **Absolute Quantification of Polysaccharides in Mushrooms using LC-MS/MS Platform; Sophia Jiang<sup>1</sup>; Shawn Ehlers-Cheang<sup>2</sup>; Christopher Suarez<sup>2</sup>; Katherine Phillips<sup>3</sup>; Naomi Fukagawa<sup>4</sup>; Carlito B. Lebrilla<sup>2</sup>; <sup>1</sup>*University***

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- of California, Davis, Davis, CA; <sup>2</sup>University of California Davis, Davis, CA; <sup>3</sup>Virginia Tech, Blacksburg, Virginia; <sup>4</sup>Beltsville Human Nutrition Research Center, Beltsville, Maryland
- MP 227 **Royal jelly's phenolic profile via UPLC-VIP-HESI-TIMS-QTOF-MS: A thorough characterization following a multivariate optimization approach;** Elena S. Nastou<sup>1</sup>; Dafni V. Preza-Mayo-Kataki<sup>1</sup>; Panagiotis- Loukas P. Gialouris<sup>1</sup>; Carsten Baessmann<sup>2</sup>; Nikolaos S. Thomaidis<sup>1</sup>; <sup>1</sup>National and Kapodistrian University of Athens, Department of Chemistry, Laboratory of Analytical Chemistry, Athens, Greece; <sup>2</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- MP 228 **Development of a Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) Targeted Screening Method for Food Additives;** Jessica K Beekman<sup>1</sup>; Katherine Carlos<sup>1</sup>; <sup>1</sup>U.S. Food and Drug Administration, Center for Food Safety and Applied Nutrition, 5001 Campus Drive, College Park, MD
- MP 229 **Give it Your All or Just 80%?: The Impact of Resuspension Solvent Composition for Standardized Nontargeted Metabolomics Analysis of Food;** Margaret Read<sup>1</sup>; Melanie T Odenkirk<sup>1</sup>; Jacqueline Michelle Chaparro<sup>1</sup>; Sahar B Toulabi<sup>1</sup>; Corey D Broeckling<sup>1</sup>; Cole Michel<sup>2</sup>; Arpana Vaniya<sup>3</sup>; Katrina Doenges<sup>2</sup>; Sarah Brinkley<sup>4</sup>; Katrina L Leaprot<sup>5</sup>; Stacy D Sherrod<sup>6</sup>; Jody C May<sup>5</sup>; Nathan Montgomery<sup>1</sup>; Richard Reisdorph<sup>2</sup>; Nichole Reisdorph<sup>2</sup>; John A McLean<sup>5</sup>; Oliver Fiehn<sup>3</sup>; Chi-Ming Chen<sup>6</sup>; Tracy Shafizadeh<sup>6</sup>; Steve Watkins<sup>6</sup>; Jessica E Prenni<sup>1</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO; <sup>2</sup>University of Colorado, Anschutz Medical Campus, Department of Pharmaceutical Sciences, Aurora, CO; <sup>3</sup>University of California Davis, Davis, CA; <sup>4</sup>The Alliance of Bioversity International & The International Center for Tropical Agriculture (CIAT), Cali, Colombia; <sup>5</sup>Vanderbilt University, Nashville, TN; <sup>6</sup>Verso Biosciences, Davis, CA
- MP 230 **Direct Analysis in Real-Time with High Resolution Mass Spectrometry: A Rapid Tool for Black Truffle Authentication;** Ilona Nordhorn<sup>1</sup>; Klemens Losso<sup>2</sup>; Matthias Rainer<sup>3</sup>; John (Jay) Brann<sup>4</sup>; Carsten Baessmann<sup>1</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>2</sup>MCI | The Entrepreneurial School, Innsbruck, Austria; <sup>3</sup>Leopold-Franzens University of Innsbruck, Innsbruck, Austria; <sup>4</sup>Bruker Daltonics GmbH & Co. KG, Billerica, MA
- MP 231 **Fabric Phase Sorptive Extraction method for the determination of veterinary drugs, pesticides and mycotoxin in milk by LC-HRMS;** Belete E Gebreyohannes<sup>1</sup>; Simiso Dube<sup>1</sup>; Mathew MM Nindi<sup>1</sup>; <sup>1</sup>University of South Africa, Florida Park, Roodepoort, South Africa
- MP 232 **Quantification of Hop-Derived Bitter Compounds in Beer Using Liquid Chromatography Mass Spectrometry;** Chieh-En Teng<sup>1</sup>; Yumeng Wang<sup>1</sup>; Tai-Huan Li<sup>2</sup>; Sung-Fang Chen<sup>1</sup>; <sup>1</sup>National Taiwan Normal University, Taipei, Taiwan; <sup>2</sup>Zhangmen Brewing Company, New Taipei City, Taiwan
- MP 233 **Simultaneous analysis of organophosphate flame retardants in food samples by LC-MS/MS;** Taek Gu Han<sup>1</sup>; Eun Seon Jeong<sup>1</sup>; Jong Seong Kang<sup>1</sup>; Hyung Min Kim<sup>1</sup>; <sup>1</sup>College of Pharmacy, chungnam University, Daejeon, South Korea
- MP 234 **Quantitation of alpha lactalbumin and beta lactoglobulin in infant formula and milk products;** Jeff Shippar; Eurofins, Madison, WI
- MP 235 **Application of untargeted headspace solid-phase microextraction-gas chromatography-mass spectrometry for volatile metabolomics-based authentication of plant-based milk alternatives;** Tianqi Li<sup>1</sup>; Renato Handoyo<sup>1</sup>; Enea Pagliano<sup>2</sup>; Yaxi Hu<sup>3</sup>; <sup>1</sup>Carleton University, Ottawa, ON; <sup>2</sup>National Research Council of Canada, Ottawa, ON; <sup>3</sup>Carleton University, Department of Chemistry, Ottawa, ON
- MP 236 **Identifying Allergen ELISA Target Proteins using Mass Spectrometry;** Ellenor R Sell<sup>1</sup>; Justin T Marsh<sup>2</sup>; Joseph L Baumert<sup>2</sup>; Philip E Johnson<sup>2</sup>; <sup>1</sup>University of Nebraska - Lincoln, Lincoln, NE; <sup>2</sup>Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, Nebraska, Lincoln, NE
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- MP 238 **Comparative analysis of electron-based fragmentation for PTM analysis in bottom-up and top-down proteomics across vendor-specific and research grade instruments;** Richard M Searfoss<sup>1</sup>; Axe Xie<sup>1</sup>; Emily Zahn<sup>1</sup>; Zongtao Lin<sup>1</sup>; Benjamin A Garcia<sup>1</sup>; <sup>1</sup>Washington University School of Medicine, Saint Louis, MO
- MP 239 **Photoactivated radical induced dissociation is sensitive to gas phase protein structure;** Brielle L Van Orman<sup>1</sup>; Ryan R. Julian<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- MP 240 **Mechanism and application of mass spectrometry fragment generation of B-type procyanidin dimers;** Kuok Fai Li<sup>1</sup>; Pai-Chi Syue<sup>1</sup>; Yao-Yuan Chuang<sup>2</sup>; Kuo-Lung Ku<sup>1</sup>; <sup>1</sup>National Chiayi University, Chiayi City, Taiwan; <sup>2</sup>National University of Kaohsiung, Kaohsiung City, Taiwan
- MP 241 **Effect of “Fixed” Negative Charges in Peptide Anion Tandem Mass Spectrometry;** Teresa Lee<sup>1</sup>; Steven A. DeFiglia<sup>1</sup>; Kristina Håkansson<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- MP 242 **Unraveling the Mysteries of Intrinsic Electron-Based Fragmentation of Cytochrome c: Insights from Species Variability;** Sarah Brandner<sup>1</sup>; Tanja Habeck<sup>1</sup>; Frederik Lermyte<sup>1</sup>; <sup>1</sup>Technical University of Darmstadt, Clemens-Schöpfung-Institute for Organic Chemistry and Biochemistry, Darmstadt, Germany
- MP 243 **Revisiting Rayleigh Instability: Unveiling the Fission Dynamics of Charged Aqueous Nanodrops Using Charge Detection Mass Spectrometry;** Veena S Avadhani<sup>1</sup>; Zachary M Miller<sup>1</sup>; Matthew S McPartlan<sup>1</sup>; Evan R Williams<sup>1</sup>; <sup>1</sup>University of California, Berkeley, Berkeley, CA
- MP 244 **Investigating the Utility of Ion Mobility-Enhanced Multistep Collisional Activation for Free Radical Initiated Peptide Sequencing (FRIPS);** Kemi E. Osho<sup>1</sup>; Nicholas B. Borotto<sup>1</sup>; <sup>1</sup>University of Nevada, Reno, RENO, NV
- MP 245 **Characterizing HDACi Interactions with Platinum by Collision-Induced Dissociation Tandem Mass Spectrometry;** Rabeva Bosri<sup>1</sup>; Qinliang Zhao<sup>2</sup>; <sup>1</sup>University of the Pacific, Stockton, CA; <sup>2</sup>University of The Pacific, Stockton, CA
- MP 246 **Analysis of surface-induced dissociation of large droplets formed by ESI in wall collisions via molecular dynamics simulations;** Michelle Rajkovic<sup>1</sup>; Walter Wißdorf<sup>1</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany
- MP 247 **Complex-Up Characterization of the Ribosome by Infrared Multiphoton Dissociation and Charge Detection Mass Spectrometry;** Sachin Tennakoon<sup>1</sup>; Mashiyat Mubassera<sup>1</sup>; Jared B. Shaw<sup>1</sup>; <sup>1</sup>University of Nebraska - Lincoln, Lincoln, NE
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**Elucidation of Saturated Hydrocarbon-derived Ketene and Acylium Ions Using Gas Chromatography Atmospheric Pressure Chemical Ionization High Resolution Mass Spectrometry; Lindsay P Brown<sup>1</sup>; Joshua B. Powers<sup>1</sup>; Shawn R. Campagna<sup>1</sup>; <sup>1</sup>University of Tennessee Knoxville Chemistry Dept., Knoxville, TN**
- MP 250 **Dehydrogenation of N-Heterocycles by [Fp]<sup>+</sup> and [CpFe(CO)]<sup>+</sup>; Robert S King<sup>1</sup>; Richard O'Hair<sup>2</sup>; Allan Canty<sup>3</sup>; John Sailor<sup>1</sup>; Victor Ryzhov<sup>1</sup>; <sup>1</sup>Northern Illinois University, Dekalb, IL; <sup>2</sup>The University of Melbourne, Melbourne, Australia; <sup>3</sup>University of Tasmania, Hobart, Australia**
- MP 251 **Optimizing Differentiation of Glycosyl Phosphate Isomers via Tandem Mass Spectrometry: Efficacy of Quasimolecular Ion vs. Fragmentation Patterns vs. Survival Yields; Nicholas M. R. Frieler<sup>1,2</sup>; Mary T Rodgers<sup>3</sup>; <sup>1</sup>Wayne State University, Detroit, MI; <sup>2</sup>University of Michigan, Ann Arbor, Michigan; <sup>3</sup>Wayne State University, Detroit, MI**
- MP 252 **Effective Acidities of Isomeric Asp-PolyPro Peptides in the Gas-Phase and in Solution; Kim Harvey<sup>1</sup>; Yadwinder Singh Mann<sup>1</sup>; Drew Wessels<sup>1</sup>; Carmen Ochoa<sup>1</sup>; Jianhua Ren<sup>1</sup>; <sup>1</sup>University of the Pacific, Stockton, CA**
- MP 253 **Ion Mobility Mass Spectrometry Reveals Changes in the Size of Metal Chalcogenide Clusters Induced by Atom-by-atom Incorporation; Xilai Li<sup>1</sup>; Hong Fang<sup>2</sup>; Dylan Forbes<sup>1</sup>; Habib Ranjbar Gholipour<sup>1</sup>; Puru Jena<sup>3</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>Purdue University Department of Chemistry, West Lafayette, IN; <sup>2</sup>Department of Physics, Rutgers University, Camden, NJ; <sup>3</sup>Department of Physics, Virginia Commonwealth University, Richmond, VA**
- MP 254 **Real-time identification and quantitation of ethylene oxide through selective gas-phase ion-molecule chemistry; Stefan J Swift<sup>1,2</sup>; Kseniya Dryahina<sup>1</sup>; Ann-Sophie Lehnert<sup>3</sup>; Nicholas Demarais<sup>4</sup>; Vaughan S. Langford<sup>4</sup>; Mark J. Perkins<sup>5</sup>; Leslie P. Silva<sup>6</sup>; Maroua Omezzine Gnious<sup>1,7</sup>; Patrik Spanel<sup>1</sup>; <sup>1</sup>J Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic; <sup>2</sup>Current Affiliation: University of Oslo, Oslo, Norway; <sup>3</sup>Syft Technologies, Darmstadt, Germany; <sup>4</sup>Syft Technologies, Christchurch, New Zealand; <sup>5</sup>Element Lab Solutions, Cambridge, United Kingdom; <sup>6</sup>Syft Technologies, Anaheim, CA; <sup>7</sup>Charles University, Prague, Czech Republic**
- MP 255 **Gas-phase Acidity of D/L-Cysteine-Containing Oligopeptides by Computational and Mass Spectrometry Studies; Shiyuan Wang<sup>1</sup>; Yuntao Zhang<sup>1</sup>; Jianhua Ren<sup>1</sup>; <sup>1</sup>University of the Pacific, Stockton, CA**
- MP 256 **Elucidation of the Zn(II) affinity of a peptide model of a Zinc finger motif from competitive threshold collision-induced dissociation; Richmond A Adomako<sup>1</sup>; Michael B Owusu<sup>2</sup>; Laurence A Angel<sup>2</sup>; <sup>1</sup>Texas A&M University-Commerce, Commerce, TX; <sup>2</sup>Texas A&M University - Commerce, Commerce, TX**
- MP 257 **Investigating the Structures of the C4H7<sup>+</sup> Cation by Cryogenic Infrared (IR) Action Spectroscopy and Electronic Structure Methods; Maleesha T Fernando<sup>1</sup>; Miyuru M Wellalage<sup>1</sup>; Katja Ober<sup>2</sup>; América Y Torres-Boy<sup>2</sup>; Madeline Schultz<sup>1</sup>; Gert von Helden<sup>2</sup>; Daniel A Thomas<sup>1</sup>; <sup>1</sup>University of Rhode Island Chemistry Department, Kingston, Rhode Island; <sup>2</sup>Fritz Haber Institute of the Max Planck Society, Berlin, Germany**
- MP 258 **Nitrile Imines as Novel Photo-Cross-Linkers for Peptides and Oligonucleotides in Gas-Phase Ions; Jiahao Wan<sup>1</sup>; Marianna Nytko<sup>2</sup>; Haocheng Qian<sup>3</sup>; Kim Vu<sup>3</sup>; Karel Lemr<sup>2,4</sup>; František Tureček<sup>3</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Department of Analytical Chemistry, Faculty of Science, Palacky University, 17. listopadu 12, Olomouc, Czech Republic; <sup>3</sup>University of Washington, Seattle, WA; <sup>4</sup>Institute of Microbiology of the Czech Academy of Sciences, Prague, Czech Republic**
- MP 259 **pH dependence of Ni(II) and Zn(II) affinities of alternative metal binding peptides from competitive threshold collision-induced dissociation; Laurence Angel<sup>1</sup>; Perfect Asare<sup>1</sup>; Kwabena N. Senyah<sup>1</sup>; Jonathan D. Wilcox<sup>1</sup>; Jovany Morales<sup>1</sup>; Riccardo Spezia<sup>2</sup>; <sup>1</sup>Texas A&M University - Commerce, Commerce, TX; <sup>2</sup>Laboratoire de Chimie Théorique, Sorbonne Université, Paris, France**
- MP 260 **Towards Annotating the Structural Heterogeneity of Model Proteins Using Gas-Phase Hydrogen/Deuterium Exchange Within an Atmospheric Pressure IM-Orbitrap Platform; Haley M Schramm<sup>1</sup>; Brian H Clowers<sup>1</sup>; <sup>1</sup>Washington State University Department of Chemistry, Pullman, WA**
- MP 261 **Fun-Source Reactivity Mass Spectrometry: Revealing Reactive Species through High-Resolution Characterization; Bessem BRAHIM<sup>1</sup>; Alban HUTEAU<sup>1</sup>; Thierry LEGOUPI<sup>1</sup>; <sup>1</sup>Shimadzu, Noisiel, France**
- MP 262 **Further Exploration of the Intrinsic Behavior of U(III) and U(IV) Complex Ions: Reactions with Iodoethane, Iodopropanes and Vinyl Iodide; Samuel J Lenze<sup>1</sup>; Michael J Van Stipdonk<sup>1</sup>; <sup>1</sup>Duquesne University, Pittsburgh, PA**
- MP 263 **Cyanocyclopentadiene Annulated Polycyclic Aromatic Radical Anions: Isomer-specific Negative Ion Photoelectron Spectra and Thermochemistry Cyanoindene and Cyanofluorene Radical Anions; Wilson Gichuhi<sup>1</sup>; Dushmantha N. Koku Hannadige Abeysooriya<sup>1</sup>; Nolan J White<sup>1</sup>; <sup>1</sup>Tennessee Tech University, Cookeville, TN**

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- MP 264 **Understanding Water Adduction to Lithiated Cannabinoids; Conner J. Baucom<sup>1</sup>; Shubin Liu<sup>1</sup>; Gary L. Glish<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC**
- MP 265 **Masked Reactivity of Hydration Clusters of Monovalent Manganese Ion: Water Insertion versus Nitrous Oxide Activation — A DFT Investigation; Chi-Kit Andy Siu; City University of Hong Kong, Hong Kong, Hong Kong**
- MP 266 **Accelerating gas-phase simulations of large proteins with the fast multipole model; Louise J Persson<sup>1</sup>; Erik G Marklund<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden**
- MP 267 **Exploring Oligomerization of Liraglutide: An Integrative Approach Using Ion Mobility Mass Spectrometry, Molecular Dynamics, and Statistic Methods; Zhenyu Xi<sup>1</sup>; Syuan-Ting Kuo<sup>1</sup>; David H Russell<sup>1</sup>; <sup>1</sup>TAMU, College Station, TX**
- MP 268 **Exploring the Influence of Microsolvation on the Conformational Landscape of Deprotonated Peptides: Computational Investigation of Leucine Enkephalin and Diserinol Isophthalamide; Nwanne D Banor<sup>1</sup>; Madeline Schultz<sup>1</sup>; Maleesha T Fernando<sup>1</sup>; Miyuru M Madduma Wellalage<sup>1</sup>; Daniel A Thomas<sup>1</sup>; <sup>1</sup>University of Rhode Island Chemistry Department, Kingston, Rhode Island**
- MP 269 **Investigating the Correlation between Bimodal CSDs of a Protein and its Behavior During the Desolvation Process using Molecular Dynamics Simulations; Samira Hajian Foroushani<sup>1</sup>; Daud Sharif<sup>1</sup>; Stephen J Valentine<sup>1</sup>; <sup>1</sup>West Virginia University, Morgantown, WV**

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- MP 270 **Ultra-Sensitive LC-MRM Based Method for Rapid and High-Throughput Screening of Sugar Phosphate Isomers in Cell Culture; Fatemeh Mousavi<sup>1</sup>; Vijay Kumar<sup>2</sup>; Jingwen Yue<sup>1,3</sup>; Dan Su<sup>1,3</sup>; <sup>1</sup>HD Biosciences, San Diego, CA; <sup>2</sup>University of Colorado, Aurora, CO; <sup>3</sup>WuXi AppTec, SAN DIEGO, California**
- MP 271 **De novo determination of fucose linkages in N-glycans and the unusual fucosylated N-glycans in insect; Chi-Kung Ni; Academia Sinica, Taipei, Taiwan**



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- MP 272 **Comparative Analysis of Milk Oligosaccharides via LC-MS: Assessing production in milk from globally distributed breeds and endangered Nordic cows;** Yu Wang<sup>1</sup>; Yu-Ping Huang<sup>1</sup>; Daniela Barile<sup>1</sup>; Heidi Leskinen<sup>2</sup>; Päivi Soppela<sup>3</sup>; Anne Tuomivaara<sup>3</sup>; <sup>1</sup>Food Science and Technology, University of California, Davis, California; <sup>2</sup>Natural Resources Institute Finland, Jokioinen, Finland; <sup>3</sup>University of Lapland, Arctic Centre, Rovaniemi, Finland
- MP 273 **Lectin-based SP3 Technology Enables N-glycoproteomics Analysis of Low Amount of Samples;** Yueshuai Guo<sup>1</sup>; Zian Huo<sup>1</sup>; Haixia Tu<sup>1</sup>; Xiangzheng Zhang<sup>1</sup>; Xuejiang Guo<sup>1</sup>; <sup>1</sup>State Key Laboratory of Reproductive Medicine and Offspring Health, Nanjing Medical University, Nanjing, China
- MP 274 **The Integration of Comprehensive Glycomic Profiling and Proteomic Analysis to Discern Unique Quality Attributes in Various Cell Therapeutics;** In-Seok Yeo<sup>1,2</sup>; Myung Jin Oh<sup>1,2</sup>; Sol Kim<sup>1,2</sup>; Jae-Young Kim<sup>1</sup>; Hyun Joo An<sup>1,2</sup>; <sup>1</sup>Chungnam National University, Daejeon, South Korea; <sup>2</sup>Asia-Pacific Glycomics Reference Site, Daejeon, South Korea
- MP 275 **Deciphering Glycosylation Changes in Glycoengineered Xenograft Models Using Glycocentric-Omics;** Myung Jin Oh<sup>1,2</sup>; Ji Eun Park<sup>1,2</sup>; Jae Ho Kim<sup>1,2</sup>; Joohyun Shim<sup>3</sup>; Kimyung Choi<sup>3</sup>; Hyun Joo An<sup>1,2</sup>; <sup>1</sup>Chungnam National University, Daejeon, South Korea; <sup>2</sup>Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; <sup>3</sup>Optipharm Inc., Chungcheongbuk-do, South Korea
- MP 276 **18-plex isobaric labeling and field asymmetric waveform ion mobility spectrometry (FAIMS)-MS enable deep N-glycomics profiling and high-throughput relative quantification;** Zicong Wang<sup>1</sup>; Lingjun Li<sup>2,3</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI; <sup>2</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- MP 277 **Boosting Quantification of N-Glycans by Enhanced Isobaric Multiplex Reagents for Carbonyl-Containing Compound (SUGAR) Tagging Strategy;** Jingwei Zhang<sup>1</sup>; Zicong Wang<sup>1</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI
- MP 278 **From Alpha to Omicron: Comparative O-Glycome Analysis of SARS-CoV-2 Spike Protein S1 by LC-MS/MS;** Parisa Ahmadi<sup>1</sup>; Vishal Sandilya<sup>1</sup>; Peilin Jiang<sup>1</sup>; Oluwatosin Daramola<sup>1</sup>; Judith Nwaiwu<sup>1</sup>; Arvin Safarian Delkosh<sup>1</sup>; Mojgan Atashi<sup>1</sup>; Mojibola Fowowe<sup>1</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, Texas
- MP 279 **Resolving Isomeric Saccharides using High Performance Liquid Chromatography Coupled to Contained Electrospray Ionization Mass Spectrometry (HPLC-cESI-MS);** Santosh Raman Acharya<sup>1</sup>; Abraham Badu-Tawiah<sup>1</sup>; <sup>1</sup>The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH
- MP 280 **An Innovative Method for Analyzing IgG Glycosylation Significance in Traumatic Brain Injury;** Sherifdeen B Onigbinde<sup>1</sup>; Joy Solomon<sup>1</sup>; Vishal Sandilya<sup>1</sup>; Oluwatosin E Daramola<sup>1</sup>; Mojibola Fowowe<sup>1</sup>; Moyinoluwa Adeniyi<sup>1</sup>; Firas Kobeissy<sup>2</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, Texas; <sup>2</sup>Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA
- MP 281 **In vitro Stable Labeling (GlyProSILC) of Mitochondria Glycans and Proteins: Unveiling Hidden Sugars in Organelles;** Judith Ijeoma Nwaiwu<sup>1</sup>; Peilin Jiang<sup>1</sup>; Oluwatosin E Daramola<sup>1</sup>; Miriam Mechref<sup>1</sup>; Odunayo O. Oluokun<sup>1</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, Texas
- MP 282 **Mass Spectrometry-Based N-Glycan Profiling of the Crustacean Neuroendocrine System;** Angel E. Ibarra<sup>1</sup>; Jingwei Zhang<sup>1</sup>; Wenxin Wu<sup>1</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, WI; <sup>2</sup>University of Wisconsin-Madison School of Pharmacy, Madison, WI
- MP 283 **Developing novel in-house packed diamond column for separation of polysaccharides based on theoretical predication;** Jyun-Ting Lin<sup>1,2</sup>; Chein-Hung Chen<sup>1</sup>; Ya-Ping Lin<sup>1</sup>; Chia-Lin Wu<sup>1</sup>; Jung-Lee Lin<sup>1</sup>; <sup>1</sup>Genomics Research Center Academia Sinica, Taipei, Taiwan; <sup>2</sup>National Cheng Kung University, Tainan, Taiwan
- MP 284 **Proteomic Insights into the Interplay between p97 and N-Glycan Profiles in Cancer Cells;** Chia Yen Liew<sup>1,2</sup>; Tsui-Fen Chou<sup>1,2</sup>; <sup>1</sup>Biology and Biological Engineering, California Institute of Technology, Pasadena, CA; <sup>2</sup>Proteome Exploration Laboratory, Beckman Institute, California Institute of Technology, Pasadena, CA
- MP 285 **Profiling N- and O-glycosylation in pancreatic juices for earlier detection of pancreatic cancer among high-risk individuals;** Yuri Van Der Burgt<sup>1</sup>; Tao Zhang<sup>1</sup>; Jihane Meziani<sup>2</sup>; Oleg A. Mayboroda<sup>1</sup>; Djuna L. Cahen<sup>2</sup>; Gwenny M. Fuhler<sup>2</sup>; Maikel P. Peppelenbosch<sup>2</sup>; Marco J. Bruno<sup>2</sup>; Manfred Wuhrer<sup>1</sup>; <sup>1</sup>Leiden University Medical Center, Leiden, Netherlands; <sup>2</sup>Erasmus Medical Center, Rotterdam, Netherlands
- MP 286 **Defining the Severity of Traumatic Brain Injury Using LC-MS/MS Glycomics of Biofluids;** Joy O Solomon<sup>1</sup>; Cristian D Gutierrez-Reyes<sup>1</sup>; Sherifdeen B Onigbinde<sup>1</sup>; Moyinoluwa Adeniyi<sup>1</sup>; Mojibola Fowowe<sup>1</sup>; Md Mostofa Al Amin Bhuiyan<sup>1</sup>; Oluwatosin E Daramola<sup>1</sup>; Judith Ijeoma Nwaiwu<sup>1</sup>; Firas Kobeissy<sup>2</sup>; Stefania Mondello<sup>3</sup>; Ava M Puccio<sup>4</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA; <sup>3</sup>Department of Biomedical and Dental Sciences and Morphofunctional Imaging, University of Messina, Messina, Italy; <sup>4</sup>Department of Neurological Surgery, University of Pittsburgh, Pittsburgh, PA
- MP 287 **Paediatric IgA Vasculitis: An LC-FAIMS-ETHcd-MS/MS O-glycan pipeline;** Andrew Chetwynd<sup>1</sup>; Claire E. Eyers<sup>2</sup>; Louise Oni<sup>2,3</sup>; <sup>1</sup>University of Liverpool, Liverpool, United Kingdom; <sup>2</sup>Liverpool University, Liverpool, United Kingdom; <sup>3</sup>Alder Hey Children's Hospital, Liverpool, United Kingdom
- MP 288 **Glycome Profiling of Small Extracellular Vesicle N-glycans as Disease Biomarkers: A Traumatic Brain Injury Case Study;** Esther O. Oji<sup>1</sup>; Mojibola Fowowe<sup>1</sup>; Moyinoluwa Adeniyi<sup>1</sup>; Ayobami Oluokun<sup>1</sup>; Oluwatosin E Daramola<sup>1</sup>; Angel J Garcia<sup>1</sup>; Cristian Gutierrez-Reyes<sup>1</sup>; Firas Kobeissy<sup>2</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA
- MP 289 **Serum N-Glycan Alterations in Rats Chronically Exposed to Glyphosate-Based Herbicide;** Favour M Chukwubueze<sup>1</sup>; Moyinoluwa Adeniyi<sup>1</sup>; Cristian D Gutierrez-Reyes<sup>1</sup>; Jesús Chávez-Reyes<sup>2</sup>; Bruno A Marichal-Cancino<sup>2</sup>; Joy O Solomon<sup>1</sup>; Mojibola O Fowowe<sup>1</sup>; Sherifdeen B Onigbinde<sup>1</sup>; Md Mostofa Al Amin Bhuiyan<sup>1</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>Department of Physiology and Pharmacology, Center of Basic Sciences, Universidad Autónoma de Aguascalientes, Aguascalientes, Mexico
- MP 290 **Characterization and quantification of mono/oligo/polysaccharides naturally occurring in pomegranate mesocarp via microfluidic chip-Q-TOF and QQQ platforms;** Han Peng<sup>1</sup>; Daniela Barile<sup>1</sup>; Nitin Nitin<sup>1</sup>; Bruna Paviani<sup>1</sup>; Yu-Ping Huang<sup>1</sup>; Nitya Raisinghani<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA
- MP 291 **Advancing Glycomics in High Grade Gliomas: A MIBI-TOF and MALDI Imaging Integrated Approach;** Mikaela Ribi<sup>1</sup>; Hadeesha Piyadasa<sup>1</sup>; Davide G. Franchina<sup>1</sup>; Ke Leow<sup>1</sup>; Meelad Amouzgar<sup>1</sup>; Benjamin Oberlton<sup>1</sup>; Richard R Drake<sup>2</sup>; Carolyn R. Bertozzi<sup>1</sup>; Sean Bendall<sup>1</sup>; Mike Angelo<sup>1</sup>; <sup>1</sup>Stanford University, Stanford, CA; <sup>2</sup>Medical University of South Carolina, Charleston, SC
- MP 292 **A novel, high-accuracy glucose-unit based N-glycan retention library and peak assignment tool for**

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- compound identification in LC or LC/MS data; Randall Robinson<sup>1</sup>; Tom Rice<sup>1</sup>; Steven Mast<sup>1</sup>; Aled Jones<sup>1</sup>; Oscar Potter<sup>2</sup>; <sup>1</sup>Agilent Technologies, Folsom, CA; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- MP 293 **Mechanistic and Quantitative Insights into Protein Interactions with Glycosphingolipids in Model Membranes;** Linh Nguyen<sup>1</sup>; Ling Han<sup>1</sup>; Elena N. Kitova<sup>1</sup>; Jianing Li<sup>1</sup>; John S. Klassen<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Alberta, Edmonton, AB
- MP 294 **Rapid LC-MS Glycan Analysis Enabling Accurate Glycan Profiling for Antibody Molecules in Cell Line Development;** Sakshi Gautam<sup>1</sup>; YenRu Pan<sup>1</sup>; Tawnya Flick<sup>1</sup>; <sup>1</sup>Gilead Sciences Inc, Oceanside, CA
- MP 295 **Discovering biomarkers in host-microbe interactions in Bacterial Vaginosis;** Yasmine Bouchibti<sup>1</sup>; Carlito B. Lebrilla<sup>2</sup>; Amanda L Lewis<sup>3</sup>; <sup>1</sup>UC Davis Graduate Studies, Davis, CA; <sup>2</sup>UC Davis, Davis, CA; <sup>3</sup>UC San Diego, La Jolla, CA

### H/D EXCHANGE: HARDWARE, SOFTWARE AND METHODOLOGY 296-307

- MP 296 **Towards Selective Removal of Unwanted Proteins under H/D Exchange Quench Conditions;** Kent Robert Vosper<sup>1</sup>; Madison Turner<sup>1</sup>; Algirdas Velyvis<sup>1</sup>; Siavash Vahidi<sup>1</sup>; <sup>1</sup>University of Guelph, Guelph, ON
- MP 297 **Towards the development of an automated in vivoHDX system to probe conformational dynamics of membrane proteins;** Juan P Rincon Pabon<sup>1</sup>; Charlotte Guffick<sup>1</sup>; Argyris Politis<sup>1</sup>; <sup>1</sup>The University of Manchester, Manchester, United Kingdom
- MP 298 **A novel HDX-MS platform for analyzing protein interactions in complex biological systems;** Joel B Langford<sup>1</sup>; Mulin Fang<sup>1</sup>; Oliver Wu<sup>1</sup>; Kellye Cupp-Sutton<sup>2</sup>; Kathleen Norris<sup>3</sup>; Judith James<sup>3,4,5</sup>; Kenneth Smith<sup>3</sup>; Si Wu<sup>2</sup>; <sup>1</sup>University of Oklahoma, Norman, OK; <sup>2</sup>University of Alabama, Tuscaloosa, AL; <sup>3</sup>Department of Arthritis and Clinical Immunology, Oklahoma Medical Research Foundation, Oklahoma City, OK; <sup>4</sup>Department of Microbiology and Immunology, Oklahoma Medical Research Foundation, Oklahoma City, OK, United States, Oklahoma City, OK; <sup>5</sup>Department of Medicine and Pathology, Oklahoma Medical Research Foundation, Oklahoma City, OK, United States, Oklahoma City, OK
- MP 299 **Advancements in MALDI for Hydrogen Deuterium Exchange Mass Spectrometry: A Systematic Evaluation;** Taylor A Murphree<sup>1</sup>; Miklos Guttman<sup>2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA
- MP 300 **HDXWizard: a software for customizable hydrogen deuterium exchange data visualization;** Zachary A. Cohen<sup>1</sup>; Bindu Y. Srinivasu<sup>1</sup>; Daniele Peterle<sup>1</sup>; John R. Engen<sup>1</sup>; Thomas E. Wales<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA
- MP 301 **Scaling HX-DIA to high throughput experimentation by replacing manual validation with statistical methods;** Vladimir Sarpe<sup>1</sup>; Jürgen Claesen<sup>2</sup>; František Filandr<sup>1</sup>; Arthur Semague<sup>1</sup>; Joey Sheff<sup>3</sup>; David C. Schriemer<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, AB; <sup>2</sup>Amsterdam University Medical Center, Amsterdam, Netherlands; <sup>3</sup>National Research Council of Canada, Ottawa, ON
- MP 302 **Leveraging cyclic ion mobility to enhance hydrogen/deuterium exchange-mass spectrometry analyses of membrane proteins within native-like lipid environments;** Damon Griffiths<sup>1</sup>; Malcolm Anderson<sup>2</sup>; Keith G Richardson<sup>2</sup>; Charlotte Guffick<sup>1</sup>; Satomi Inaba-Inoue<sup>3</sup>; Konstantinos Beis<sup>3</sup>; Mike Morris<sup>2</sup>; Kevin Giles<sup>2</sup>; Argyris Politis<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, United Kingdom; <sup>2</sup>Waters Corporation, Manchester, United Kingdom; <sup>3</sup>Imperial College London, London, United Kingdom

- MP 303 **Optimization of Instrument Parameters for HX-DIA with AutoHX;** Maryam Hassannia<sup>1</sup>; František Filandr<sup>1</sup>; David C. Schriemer<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, AB
- MP 304 **Determining EX1 protein unfolding kinetics in library scale HDX experiments;** Jane Thibeault<sup>1</sup>; Allan J. R. Ferrari<sup>1</sup>; Gabriel Rocklin<sup>1</sup>; <sup>1</sup>Northwestern University, Feinberg School of Medicine, Chicago, IL
- MP 305 **Streamlined Software Approach for Controlling Modules in a Mass Spectrometer;** Francis E. Godfrey<sup>1</sup>; Michael Eller<sup>1</sup>; <sup>1</sup>Cal State Northridge, Northridge, CA
- MP 306 **Reducing gas-phase hydrogen/deuterium scrambling on a QTOF Mass Spectrometer equipped with electron activated dissociation (EAD) fragmentation technology;** Joseph Anacleto<sup>1</sup>; Ebadullah Kabir<sup>2</sup>; Yves LeBlanc<sup>3</sup>; Cristina Lento<sup>2</sup>; Derek J. Wilson<sup>2</sup>; <sup>1</sup>Emeritus, Brampton, ON; <sup>2</sup>York University, Toronto, ON; <sup>3</sup>SCIEX, Concord, ON
- MP 307 **Probe the Protein Conformation using Top-down Hydrogen Exchange Mass Spectrometry at Higher Resolution with Electron Transfer Dissociation;** Yuj Shi<sup>1</sup>; Graeme McAlister<sup>1</sup>; Rosa Viner<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA

### H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION 308-338

- MP 308 **HDX-MS insights into the conformational and oligomeric heterogeneity of PafA, the mycobacterial prokaryotic ubiquitin-like protein (Pup) ligase;** Alicia Plourde<sup>1</sup>; Jacquelyn Ogata-Bean<sup>1</sup>; Siavash Vahidi<sup>1</sup>; <sup>1</sup>University of Guelph, Guelph, ON
- MP 309 **Substrate engagement mechanism of an ATP-independent proteasome activator from Mycobacterium tuberculosis: Insights from HDX and native MS;** Bradley Davis<sup>1</sup>; Algirdas Velyvis<sup>1</sup>; Siavash Vahidi<sup>1</sup>; <sup>1</sup>University of Guelph, Guelph, ON
- MP 310 **Investigating the role of allostery in the regulation of human mitochondrial ClpP: implications for the treatment of acute myeloid leukemia;** Monica M Goncalves<sup>1</sup>; Adwaith B. B. Uday<sup>2</sup>; Ian Watson<sup>3</sup>; S. Quinn W. Currie<sup>1</sup>; Taylor Forrester<sup>1</sup>; Angelina S. Kim<sup>1</sup>; Algirdas Velyvis<sup>1</sup>; Matthew Kimber<sup>1</sup>; Rima Al-Awar<sup>2</sup>; Natalie Zeytuni<sup>2</sup>; Aaron Schimmer<sup>4</sup>; Siavash Vahidi<sup>1</sup>; <sup>1</sup>University of Guelph, Guelph, ON; <sup>2</sup>McGill University, Montreal, QC; <sup>3</sup>Ontario Institute for Cancer Research, Toronto, ON; <sup>4</sup>Princess Margaret Cancer Centre, University Health Network, Toronto, ON
- MP 311 **The Unique Advantage of HDX-MS Over Traditional Structural Biology Tools: the Case of the 20S Proteasome Core Particle;** Madison Turner<sup>1</sup>; Samuel E Hoff<sup>2</sup>; Adwaith B. B. Uday<sup>3</sup>; Algirdas Velyvis<sup>1</sup>; Natalie Zeytuni<sup>3</sup>; Massimiliano Bonomi<sup>2</sup>; Siavash Vahidi<sup>1</sup>; <sup>1</sup>University of Guelph, Guelph, ON; <sup>2</sup>Institut Pasteur, Paris, France; <sup>3</sup>McGill University, Montreal, QC
- MP 312 **A Structural and Dynamic Basis for the Interactions of the Dengue Nonstructural (NS5) Protein with Stem Loop A (SLA);** Juliet Obi<sup>1</sup>; Kyle C. Kihn<sup>2</sup>; Ally K. Smith<sup>1</sup>; Linfah McQueen<sup>1</sup>; Daniel J. Deredge<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore, Baltimore, MD; <sup>2</sup>Georgetown University, Washington Dc, DC
- MP 313 **pH-dependent conformational changes and structural dynamics of Brain-Type Creatine Kinase;** Nolan K McLaughlin<sup>1</sup>; Samantha Gies<sup>2</sup>; Reza Dastvan<sup>2</sup>; Michael Gross<sup>1</sup>; <sup>1</sup>Washington University in Saint Louis, St. Louis, MO; <sup>2</sup>Saint Louis University School of Medicine, St. Louis, MO
- MP 314 **Characterization of a new class of influenza antibodies by integrating HDX-MS with computational modeling;** Minh H. Tran<sup>1</sup>; Cristina E. Martina<sup>1</sup>; Iuliia M. Gilchuck<sup>2</sup>; James E. Crowe<sup>2,3,4</sup>; Jens Meiler<sup>1,5</sup>; Kevin L. Schey<sup>6</sup>; <sup>1</sup>Department of Chemistry and Center for Structural Biology, Vanderbilt University, Nashville, TN; <sup>2</sup>Vanderbilt Vaccine Center, Vanderbilt University Medical Center, Nashville, TN; <sup>3</sup>Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; <sup>4</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical

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- Center, Nashville, TN; <sup>5</sup>Institute for Drug Discovery, University Leipzig Medical School, Leipzig, Saxony; <sup>6</sup>Department of Biochemistry and Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN
- MP 315 **Characterizing the functional role of the C-terminal extension of human mitochondrial ClpP; S. Quinn W. Currie<sup>1</sup>; Monica M. Goncalves<sup>1</sup>; Siavash Vahidi<sup>1</sup>; <sup>1</sup>University of Guelph, Guelph, ON**
- MP 316 **Innovative data-analysis method to accurately extract peptic-peptide energies of wildtype-Staphylococcal Nuclease in PEPs-HDX-MS experiments to challenge the two-state folding model; Motolani O Matthew<sup>1, 2</sup>; Rohana Liyanage<sup>1, 2</sup>; Isini Ranawake Arachchige<sup>1, 2</sup>; Wesley Stites<sup>1</sup>; Jackson O. Lay<sup>1, 2</sup>; <sup>1</sup>UNIVERSITY OF ARKANSAS, FAYETTEVILLE, AR; <sup>2</sup>Arkansas Statewide Mass Spectrometry Facility, FAYETTEVILLE, AR**
- MP 317 **Comprehensive HDX-MS Analysis is a Key Driver in Lead Selection and Characterization in Pharmaceutical Research; Cornelia Wagner<sup>1</sup>; Sarah Mundigl<sup>1</sup>; Urs Hanke<sup>1</sup>; Maximiliane Koenig<sup>1</sup>; <sup>1</sup>Roche Innovation Center Munich (RICM), Roche Pharma Research and Early Development (pRED), Penzberg, Germany**
- MP 318 **Analyzing protease inhibitors: A case study on the Coronavirus 3CL protease using an automated rapid screening and HDX-MS; Jonathan Zöller<sup>1</sup>; Frederic Farges<sup>2</sup>; Barbara Rathmann<sup>1</sup>; Joshua Vollrath<sup>1</sup>; Nadide Altincekic<sup>3, 4</sup>; Kristina Desch<sup>5</sup>; Jakob Meier-Credo<sup>1</sup>; Harald Schwalbe<sup>3, 4</sup>; Ulrich Mrowietz<sup>6</sup>; Julian D. Langer<sup>1, 5</sup>; <sup>1</sup>Max Planck Institute of Biophysics, Frankfurt, Germany; <sup>2</sup>Institute of Pharmaceutical Chemistry, Johann Wolfgang Goethe University, Frankfurt am Main, Germany; <sup>3</sup>Center for Biomolecular Magnetic Resonance (BMRZ), Institute for Organic Chemistry and Chemical Biology, Goethe University, Frankfurt am Main, Germany; <sup>4</sup>Institute for Organic Chemistry and Chemical Biology, Goethe University, Frankfurt am Main, Germany; <sup>5</sup>Max Planck Institute for Brain Research, Frankfurt, Germany; <sup>6</sup>Dept. of Dermatology, University Medical Center Schleswig-Holstein, Kiel, Germany**
- MP 319 **Epitope mapping and protein dynamics analysis by HDX-MS to characterize the antigenicity maturation effect of SARS CoV-2 Beta spike protein; Shaolong Zhu<sup>1</sup>; Lisa Szymkowitz<sup>1</sup>; Jason Szeto<sup>1</sup>; Fernando Salvador Ausar<sup>1, 2</sup>; Andrew James<sup>1</sup>; Michael Leach<sup>1</sup>; <sup>1</sup>Sanofi, Toronto, ON; <sup>2</sup>Vaxcyte, San Carlos, CA**
- MP 320 **Unraveling Variations in the Dynamic Binding of PD1 between Toripalimab and other Commercial PD-1 Monoclonal Antibodies through HDX-MS Analysis; Bin Yu<sup>1</sup>; Glen Young<sup>1</sup>; <sup>1</sup>coherus bioscience, Camarillo, CA**
- MP 321 **Structural basis of DNMT3A oligomeric states in acute myeloid leukemia revealed by hydrogen-deuterium exchange (HX) and cross-linking (XL) mass spectrometry; Shaunak Raval<sup>1</sup>; Emma Garcia<sup>2</sup>; Keith Rivera<sup>1</sup>; Maya Virshup<sup>1</sup>; Brian B. Liau<sup>1, 2</sup>; Steven A. Carr<sup>1</sup>; Malvina Papanastasiou<sup>1</sup>; <sup>1</sup>Broad Institute, Cambridge, MA; <sup>2</sup>Harvard University, Cambridge, MA**
- MP 322 **Homemade quench flow apparatus enhances Protein Equilibrium Population Snapshot (PEPS-HDX-MS) applications, enabling accurate protein structure analysis through rapid sample quenching; Isini Pinipa Ranawake Arachchige<sup>1, 2</sup>; Rohana Liyanage<sup>1, 2</sup>; Motolani O Matthew<sup>1, 2</sup>; Wesley Stites<sup>1</sup>; Jackson O. Lay<sup>1, 2</sup>; <sup>1</sup>UNIVERSITY OF ARKANSAS, FAYETTEVILLE, AR; <sup>2</sup>Arkansas Statewide Mass Spectrometry Facility, FAYETTEVILLE, AR**
- MP 323 **HDX-MS of surface-bound IgM provides insight into complement cascade activation; Charles Mundorff<sup>1</sup>; Malika Hale<sup>1</sup>; Adian Valdez<sup>1</sup>; Lauren Carter<sup>1</sup>; Neil King<sup>1</sup>; David J Rawlings<sup>1</sup>; Marion Pepper<sup>1</sup>; Miklos Guttman<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA**
- MP 324 **Beyond epitope mapping: combining solid-state NMR and structural mass spectrometry to gain new insights for precision biotech development; Francesca Sacco<sup>1</sup>; Angela Capolupo<sup>2</sup>; Sofia Petrocchi<sup>3</sup>; Jonathan Zöller<sup>4</sup>; Linda Cerofolini<sup>1, 5</sup>; Julian D. Langer<sup>4, 6</sup>; Fabio Baroni<sup>3</sup>; Marco Fragai<sup>1, 5, 7</sup>; <sup>1</sup>Magnetic Resonance Center (CERM), University of Florence, Sesto Fiorentino (FI), Italy; <sup>2</sup>Analytical Development & Innovation - NBE, Merck Serono S.p.a, Guidonia (Rome), Italy; <sup>3</sup>Analytical Development & Innovation - NBE, Merck Serono S.p.a, Guidonia (Rome), Italy; <sup>4</sup>Max Planck Institute of Biophysics, Frankfurt, Germany; <sup>5</sup>Consorzio Interuniversitario Risonanze Magnetiche di Metalloproteine (CIRMMP), Sesto Fiorentino (FI), Italy; <sup>6</sup>Max Planck Institute for Brain Research, Frankfurt, Germany; <sup>7</sup>Department of Chemistry "Ugo Schiff", University of Florence, Sesto Fiorentino (FI), Italy**
- MP 325 **Hydrogen Deuterium Exchange Mass Spectrometry of the CheW Coupling Protein in E.coli Chemoreceptor Complexes; Isabella J Jankowski<sup>1</sup>; Thomas Tran<sup>1</sup>; Lynmarie K. Thompson<sup>1, 2</sup>; Steve Eyles<sup>2</sup>; <sup>1</sup>Department of Chemistry, University of Massachusetts Amherst, Amherst, MA; <sup>2</sup>Department of Biochemistry and Molecular Biology, University of Massachusetts Amherst, Amherst, MA**
- MP 326 **Impact of clinically approved BTK inhibitors on full-length BTK conformation and analysis of the development of BTK resistance mutations; Thomas E. Wales<sup>1</sup>; Raji E. Joseph<sup>2</sup>; Sandrine Jayne<sup>3</sup>; Robert G. Britton<sup>3</sup>; D. Bruce Fulton<sup>2</sup>; John R. Engen<sup>1</sup>; Martin J.S. Dyer<sup>3</sup>; Amy H. Andreotti<sup>2</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Iowa State University, Ames, IA; <sup>3</sup>University of Leicester, Leicester, United Kingdom**
- MP 327 **Spike Protein RBDs of SARS-CoV-2 Variants and their Interactions with Neutralizing Antibodies: Conformational Dynamics Revealed by Hydrogen/Deuterium Exchange Mass Spectrometry; Qinyu Jia<sup>1</sup>; Zhongping Yao<sup>2</sup>; <sup>1</sup>the Hong Kong Polytechnic University, Kowloon, Hong Kong; <sup>2</sup>The Hong Kong Polytechnic University, Kowloon, Hong Kong**
- MP 328 **Combination of HDX-MS and MD Simulations Identified Closed Conformation of the Full-Length Bcl-2; Miray Turk<sup>1</sup>; Umüt Cagan Ucar<sup>1</sup>; Baran Dingiloglu<sup>1</sup>; Yagiz Akbas<sup>1</sup>; Gizem Dinler Doganay<sup>1</sup>; <sup>1</sup>Istanbul Technical University, Istanbul, Turkey**
- MP 329 **HDX-MS reveals binding of a neutralizing antibody to TNFα allosterically interferes with its binding to TNFR1; Christopher A. Haynes<sup>1</sup>; Theodore R. Keppel<sup>1</sup>; John R. Barr<sup>1</sup>; Dongxia Wang<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA**
- MP 330 **Native MS and HDX Characterization of the Mechanism of GSTP1 Protein Glutathionylation; Xinyi Cynthia Kuang<sup>1</sup>; Heather Benedict-Hamilton<sup>2</sup>; Marta Zurawska<sup>2</sup>; Andrzej Krezel<sup>2</sup>; Jason M Held<sup>2</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>Washington University School of Medicine, St. Louis, MO**
- MP 331 **Conformational Dynamics of Glucokinase and Modulation by a Molecular Activator as Characterized by Hydrogen Deuterium Exchange Mass Spectrometry; Bindu Y. Srinivasu<sup>1</sup>; Michelle S. Prew<sup>2</sup>; Gregory H. Bird<sup>2</sup>; Nika N. Danial<sup>3</sup>; Loren D. Walensky<sup>2</sup>; John R. Engen<sup>1</sup>; Thomas E. Wales<sup>1</sup>; <sup>1</sup>Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; <sup>2</sup>Department of Pediatric Oncology and the Linde Program in Cancer Chemical Biology, Dana-Farber Cancer Institute, Boston, MA; <sup>3</sup>Departments of Cancer Biology and Medical Oncology, Dana-Farber Cancer Institute, Boston, MA**
- MP 332 **Mapping Epitopes on Borrelia burgdorferi Outer Surface Proteins by Hydrogen Deuterium Exchange Mass Spectrometry (HDX-MS); Clint Vorauer<sup>1</sup>; Beatrice Muriuki<sup>2</sup>; David Vance<sup>3</sup>; Michael Rudolph<sup>4</sup>; Lisa Cavacini<sup>5</sup>; Nicholas Mantis<sup>6</sup>; Miklos Guttman<sup>1</sup>; <sup>1</sup>University of Washington - Medicinal Chemistry, Seattle, Washington; <sup>2</sup>University of Massachusetts Boston, Boston, Massachusetts; <sup>3</sup>University at Albany, State University of New York, Albany, New York; <sup>4</sup>New York Structural Biology Center, New York, New York;**

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- <sup>5</sup>University of Massachusetts Boston, Boston, MA; <sup>6</sup>New York State Department of Health, Albany, New York
- MP 333 **MD simulations, mass spectrometry and other biophysical techniques elucidate stabilising features of a nanobody against an HIV capsid;** Valentina Faustini<sup>1</sup>; Eva Illes-Toth<sup>2</sup>; Paul Dalby<sup>1</sup>; <sup>1</sup>UCL, London, United Kingdom; <sup>2</sup>LGC, London, United Kingdom
- MP 334 **Exploring PF4 Dynamics in Thrombocytopenia: Insights from Hydrogen-Deuterium Exchange Mass Spectrometry;** Yi Du<sup>1</sup>; Daniel Heron<sup>1</sup>; Igor A. Kaltashov<sup>1</sup>; <sup>1</sup>University of Massachusetts-Amherst, Amherst, MA
- MP 335 **Broadly neutralizing humanized SARS-CoV-2 antibody binds to a conserved epitope on spike protein and provides antiviral protection through inhalation-based delivery;** Esther Wolf<sup>1</sup>; Cristina Lento<sup>1</sup>; Derek J. Wilson<sup>1</sup>; Mart Ustav Jr.<sup>2</sup>; <sup>1</sup>York University, Toronto, ON; <sup>2</sup>Icosagen Cell Factory OÜ, Tartu, Estonia
- MP 336 **Structural dynamics of botulinum neurotoxin type A from hydrogen/deuterium exchange mass spectrometry;** Heather Bottomley<sup>1</sup>; David Spencer<sup>2</sup>; Rick Beardmore<sup>2</sup>; Rachel Bostock<sup>2</sup>; Jonathan Phillips<sup>1</sup>; <sup>1</sup>University of Exeter, Exeter, United Kingdom; <sup>2</sup>Ipsen Biopharm, Wrexham, United Kingdom
- MP 337 **Characterizing Conformational Dynamics of In Vitro Hyperphosphorylated Human Tau by Time-resolved Hydrogen/Deuterium Exchange Mass Spectrometry;** Ayesha Chaudhry<sup>1</sup>; Derek J. Wilson<sup>1</sup>; <sup>1</sup>York University, Toronto, ON
- MP 338 **Standardization of HDX-MS Paratope Mapping Conditions for Monoclonal Antibodies using a Range of Acidic Proteases;** Dominic Narang<sup>1</sup>; Konrad Celejewski<sup>1</sup>; <sup>1</sup>Rapid Novor, Kitchener, Ontario
- IMAGING MS: PHARMACEUTICALS, METABOLITES, LIPIDS, AND GLYCANS I**  
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- MP 339 **Revolutionizing Spatial Dermatology: Investigating Sunfilter Efficacy on Reconstructed Human Epidermis with AP-MALDI MSI Metabolomics and Dedicated Data Analysis Software;** Sara Tortorella<sup>1</sup>; Maureen Feucherolles<sup>2</sup>; Giulia Sorbi<sup>1</sup>; Giuseppe Arturi<sup>1</sup>; Sue Kennerley<sup>3</sup>; Gilles Frache<sup>2</sup>; Ismael Zamora<sup>4</sup>; <sup>1</sup>Mass Analytica, S.L, Bettona, Italy; <sup>2</sup>Luxembourg Institute of Science and Technology, Molecular and Thermal Analysis, Belvaux, Luxembourg; <sup>3</sup>K R Analytical, Sandbach, United Kingdom; <sup>4</sup>Mass Analytica, S.L, Sant Cugat del Vallés, Spain
- MP 340 **Visualisation and quantitation of drug/metabolites by sensitive and fast targeted DESI imaging TQ system;** Emmanuelle Claude<sup>1</sup>; Ross Chawner<sup>1</sup>; Nathalie Delalée<sup>2</sup>; Stephanie Molez<sup>2</sup>; Gregory Nicolas<sup>2</sup>; Joanne Bellantyne<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Bioprojet Biotech, Saint Gregoire, France
- MP 341 **Lessons learnt from the Cancer Grand Challenge Rosetta Project– Metabolic Imaging at Scale;** Rory Thomas Steven<sup>1</sup>; Alex Dexter<sup>1</sup>; Ariadna Gonzalez<sup>1</sup>; Bin Yan<sup>1</sup>; Caroline Pollard<sup>1</sup>; Janella Marie De Jesus<sup>1</sup>; Greg McMahon<sup>1</sup>; Simon Barry<sup>2</sup>; Kevin Brindle<sup>3</sup>; George Poulgiannis<sup>4</sup>; Richard Goodwin<sup>2</sup>; Mariia Yuneva<sup>5</sup>; Owen Sansom<sup>6</sup>; Josephine Bunch<sup>1, 7</sup>; <sup>1</sup>National Physical Laboratory, London, United Kingdom; <sup>2</sup>AstraZeneca, Cambridge, United Kingdom; <sup>3</sup>Cancer Research UK Cambridge Institute, University of Cambridge, Cambridge, United Kingdom; <sup>4</sup>Institute for Cancer Research, London, United Kingdom; <sup>5</sup>Francis Crick Institute, London, United Kingdom; <sup>6</sup>CRUK Scotland Institute, Glasgow, United Kingdom; <sup>7</sup>Imperial College London, London, United Kingdom
- MP 342 **Spatially Resolved Metabolomics Reveals Tissue-Specific Metabolic Changes in the Kidney and Bladder after Cisplatin Treatment;** Jephthe Akakpo<sup>1</sup>; Erika Abbott<sup>2</sup>; Ben Woolbright<sup>3</sup>; Bindesh Shrestha<sup>4</sup>; Cory Scanlan<sup>4</sup>; Dennis Karote<sup>4</sup>; John Taylor<sup>2, 3</sup>; <sup>1</sup>Department of Pharmacology, Toxicology & Therapeutics, University of Kansas Medical Center, Kansas City, KS; <sup>2</sup>Department of Urology, University of Kansas Medical Center, Kansas City, KS; <sup>3</sup>Department of Cancer Biology, University of Kansas Medical Center, Kansas City, KS; <sup>4</sup>Waters Corporation, Milford, Massachusetts
- MP 343 **Spatial Mapping of Ether Lipids in Tissue via MALDI TIMS Imaging Mass Spectrometry: Characterization of Biomarkers of Peroxisomal Disorders;** Melanie J Campbell<sup>1</sup>; Erin H. Seeley<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>University of Texas at Austin, Austin, TX
- MP 344 **Skin and the Hair Cycle–Spatial Lipidomics Analysis of the Dermis and Epidermis as a Function of the Adipokine Adiponectin;** Katarzyna Walendzik<sup>1</sup>; Eii-Chi Matsuo<sup>2</sup>; Jeff Dahl<sup>3</sup>; Toshiya Matsubara<sup>3</sup>; Shinichi Yamaguchi<sup>2</sup>; Jannine I. Gamayot<sup>1</sup>; Philipp E Scherer<sup>1</sup>; Ruth Gordillo<sup>1</sup>; <sup>1</sup>UTSouthwestern Medical Center, Dallas, TX; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Shimadzu Scientific Instruments, Columbia, MD
- MP 345 **Mass Spectrometry Imaging Reveals Alterations in Protein and N-Glycan Molecular Signatures in Endometriosis Tissues;** Monica Lin<sup>1</sup>; Erin H. Seeley<sup>2</sup>; Suzanne Ledet<sup>3</sup>; Christina Salazar<sup>4</sup>; Michael T. Breen<sup>4</sup>; Livia S. Eberlin<sup>1</sup>; <sup>1</sup>Baylor College of Medicine, Houston, Texas; <sup>2</sup>University of Texas at Austin, Austin, Texas; <sup>3</sup>Ascension Seton Medical Center, Department of Pathology, Austin, Texas; <sup>4</sup>The University of Texas at Austin Dell Medical School, Department of Women's Health, Austin, Texas
- MP 346 **Multimodal Mass Spectrometry Imaging of Uveal Melanoma Multi-Cellular Tumour Spheroids to Investigate Key Metabolomic Biomarkers;** Georgia M Millard<sup>1</sup>; Neil A Cross<sup>1</sup>; Karen Aughton<sup>2, 3</sup>; Helen Kalirai<sup>2, 3</sup>; Laura M Cole<sup>1</sup>; <sup>1</sup>Sheffield Hallam University, Sheffield, United Kingdom; <sup>2</sup>University of Liverpool, Liverpool, United Kingdom; <sup>3</sup>Liverpool Ocular Oncology Research Group, Liverpool, United Kingdom
- MP 347 **Development of MALDI-MSI methods to detect and visualize new TB regimen drugs within TB lesions;** Bandana Bera<sup>1</sup>; Prem Shankar<sup>1</sup>; Jenny Myrick<sup>2</sup>; Meredith Bacci<sup>2</sup>; David Brown<sup>2</sup>; Arnold Louie<sup>2</sup>; George Drusano<sup>2</sup>; Brendan Prideaux<sup>1</sup>; <sup>1</sup>University Of Texas Medical Branch, Galveston, TX; <sup>2</sup>University of Florida, Department of Medicine, Orlando, FL
- MP 348 **Investigation of Microbial Metabolites and Their Potential for Impact in Early Life Immune System Development;** Troy R Scoggins IV<sup>1</sup>; Julia Flores<sup>2, 3</sup>; Joseph P. Zackular<sup>4, 5</sup>; Michael A. Silverman<sup>3, 4</sup>; Boone M. Prentice<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Florida, Gainesville, FL; <sup>2</sup>Department of Pediatrics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; <sup>3</sup>Division of Infectious Disease, Children's Hospital of Philadelphia, University of Pennsylvania, Philadelphia, PA; <sup>4</sup>Division of Protective Immunity, Children's Hospital of Philadelphia, Philadelphia, PA; <sup>5</sup>Department of Pathology and Laboratory Medicine, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA
- MP 349 **MALDI mass spectrometry imaging reveals highly localized phosphatidylcholine metabolism alterations in pancreatic tumor tissues in response to gemcitabine treatment;** Nav Raj Phulara<sup>1</sup>; Chiaki Tsuge Ishida<sup>2</sup>; Peter J. Espenshade<sup>2, 3</sup>; Herana Kamal Seneviratne<sup>1</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, University of Maryland, Baltimore County, Baltimore, MD; <sup>2</sup>Department of Cell Biology, The Johns Hopkins University School of Medicine, Baltimore, MD; <sup>3</sup>Department of Oncology, The Johns Hopkins University School of Medicine, Baltimore, MD
- MP 350 **Evaluation of anti-ENTPD2 antibody treatment in tumors using MALDI imaging mass spectrometry;** Kerri Grove<sup>1</sup>; Shailla Hoque<sup>1</sup>; Samantha Zaharevitz<sup>2</sup>; Richard Salamone<sup>2</sup>; Deborah Knee<sup>2</sup>; Shu Li<sup>3</sup>; Anthu Dang<sup>3</sup>; Patrick Rudewicz<sup>1</sup>; <sup>1</sup>Novartis, Emeryville, CA; <sup>2</sup>Novartis, San Diego, CA; <sup>3</sup>Novartis, Cambridge, MA
- MP 351 **Combining MALDI-IMS and segmentation via autofluorescence to analyze glycan speciation within**

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- specific functional tissue units in human organs;** David T. Reeves<sup>1, 2</sup>; Audra M. Judd<sup>1, 3</sup>; Lukasz Migas<sup>4</sup>; Ellie L. Pingry<sup>1, 2</sup>; Felipe A. Moser<sup>4</sup>; Jamie Allen<sup>1, 3</sup>; Angela R. S. Kruse<sup>1, 2</sup>; Melissa A. Farrow<sup>1, 3, 5</sup>; Raf Van De Plas<sup>1, 3, 4</sup>; Jeffrey M. Spraggins<sup>1, 2, 3, 5</sup>; <sup>1</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>2</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>3</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>4</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>5</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN
- MP 352 **Uncovering lipid heterogeneity in cerebral amyloid angiopathy using MALDI IMS coupled with IF microscopy;** Cody Marshall<sup>1, 2, 3</sup>; Claire F. Scott<sup>3, 4, 5</sup>; Lissa Ventura-Antunes<sup>6, 7</sup>; Wilber Romero-Fernandez<sup>7</sup>; Alena Shostak<sup>6, 7</sup>; Lukasz Migas<sup>4, 8</sup>; Madeline E. Colley<sup>3, 4, 9</sup>; Martin Dufresne<sup>3, 4, 9</sup>; Raf Van De Plas<sup>3, 4, 8</sup>; Matthew S. Schrag<sup>6, 7</sup>; Jeffrey M. Spraggins<sup>1, 3, 4, 5, 9, 10</sup>; <sup>1</sup>Chemical and Physical Biology Program, Vanderbilt University, Nashville, Tennessee; <sup>2</sup>Biomolecular Multimodal Imaging Center, Nashville, Tennessee; <sup>3</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>4</sup>Biomolecular Multimodal Imaging Center, Vanderbilt University, Nashville, TN, Nashville, Tennessee; <sup>5</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, Tennessee; <sup>6</sup>Vanderbilt University Medical Center, Nashville, TN; <sup>7</sup>Department of Neurology, Vanderbilt University, Nashville, TN; <sup>8</sup>Delft University of Technology, Delft, Netherlands; <sup>9</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>10</sup>Department of Chemistry, Vanderbilt University, Nashville, TN
- MP 353 **Comparison of Antigen Retrieval Techniques to Improve Lipidomic Analysis of Formalin-Fixed/Paraffin-Embedded Tissue in MALDI-MSI Using Canine Sarcoma Samples;** Ziven Noorani<sup>1</sup>; A. Colleen Crouch<sup>1</sup>; <sup>1</sup>University of Tennessee, Knoxville, TN
- MP 354 **Spatial metabolomics reveals accumulation of ceramides and sphingomyelins in motor neurons of lumbar spinal cords in amyotrophic lateral sclerosis;** Guanshi Zhang<sup>1</sup>; Ian M. Tamayo<sup>1</sup>; Stacey Jacoby<sup>2</sup>; Stephen Goutman<sup>2</sup>; Eva L. Feldman<sup>2</sup>; Kumar Sharma<sup>1</sup>; <sup>1</sup>UT Health San Antonio, San Antonio, TX; <sup>2</sup>University of Michigan-Ann Arbor, Ann Arbor, MI
- MP 355 **Investigating Metabolic Alterations in Neonatal Transgenic Mice Heart with Various Proliferation Capacity using Desorption Electrospray Ionization Mass Spectrometry Imaging;** Sarah Bench<sup>1</sup>; Abou Bakr M. Salama<sup>1</sup>; Tamer M. A. Mohamed<sup>1</sup>; Livia S. Eberlin<sup>1</sup>; <sup>1</sup>Baylor College of Medicine, Dept. of Surgery, Houston, Texas
- MP 356 **Applications of Mass Spectrometry-Based Platforms to Advance Drug Discovery Pipeline;** Esther Cheow<sup>1</sup>; U-Ming Lim<sup>1</sup>; Nikhil Tulsian<sup>1</sup>; Matthew Choo<sup>1</sup>; Aaron Zefrin Fernandis<sup>1</sup>; <sup>1</sup>Target & Pathway Biology, Quantitative Biosciences, MSD, Singapore, Singapore
- MP 357 **Defining lipidomic and metabolic signatures of monomicrobial and dual-species biofilms using MALDI IMS;** Alexis P. Pope<sup>1, 2</sup>; Jeffrey A. Freiberg<sup>3, 4</sup>; Lukasz Migas<sup>5</sup>; Madeline E. Colley<sup>1, 6</sup>; Raf Van De Plas<sup>5</sup>; Eric P. Skaar<sup>3, 7</sup>; Jeffrey M. Spraggins<sup>1, 2, 3, 7, 8, 9, 10</sup>; <sup>1</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>2</sup>Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN; <sup>3</sup>Vanderbilt Institute for Infection, Immunology and Inflammation, Vanderbilt University Medical Center, Nashville, TN; <sup>4</sup>Division of Infectious Diseases, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; <sup>5</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>6</sup>Vanderbilt University, Department of Biochemistry, Nashville, TN; <sup>7</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; <sup>8</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>9</sup>Department of Chemistry, Vanderbilt University, Nashville, TN; <sup>10</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN
- MP 358 **Revealing Spatial Heterogeneity at the Gut Epithelium-Lumen Interface through High-Resolution MALDI-TOF Chemical Imaging;** Jacob Haffner<sup>1</sup>; Gillian Robbins<sup>1</sup>; Soo Hyun Ahn<sup>2</sup>; Tian Autumn Qiu<sup>1</sup>; <sup>1</sup>Michigan State University, Department of Chemistry, East Lansing, MI; <sup>2</sup>Michigan State University, College of Veterinary Medicine, Department of Pathobiology and Diagnostics Investigation, East Lansing, MI
- MP 359 **Investigating long-term exposure to phthalates in patients with skin abscesses using MALDI FT-ICR MSI;** Temple Andrews<sup>1</sup>; Beita Badie<sup>2</sup>; Nina Rossa Haddad<sup>2</sup>; Hana Minsky<sup>2</sup>; Yingchao Xue<sup>2</sup>; Luis Garza<sup>2</sup>; Maureen A. Kane<sup>1</sup>; <sup>1</sup>University of Maryland School of Pharmacy, Baltimore, MD; <sup>2</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- MP 360 **Mapping Metabolites in the Human Eye: Integrating High Spatial Resolution MALDI IMS for Insights into Ocular Health;** Ali Zahraei<sup>1, 2</sup>; Martin Dufresne<sup>2, 3</sup>; David M. G. Anderson<sup>2, 3</sup>; Madeline E. Colley<sup>1, 2</sup>; Angela R. S. Kruse<sup>1, 2</sup>; Lukasz Migas<sup>4</sup>; Jeffery Messinger<sup>5</sup>; Christine A. Curcio<sup>5</sup>; Raf Van De Plas<sup>4</sup>; Kevin L. Schey<sup>2, 3</sup>; Jeffrey M. Spraggins<sup>1, 2, 3, 6, 7</sup>; <sup>1</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>2</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>3</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>4</sup>Delft University of Technology, Delft, Netherlands; <sup>5</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>6</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; <sup>7</sup>Department of Chemistry, Vanderbilt University, Nashville, TN
- MP 361 **Highly sensitive nano-DESI mass spectrometry imaging of glycolipids using ionization enhancement solvent additives;** Aiming Zheng<sup>1</sup>; Miranda Weigand<sup>2</sup>; Manxi Yang<sup>2</sup>; Julia Laskin<sup>2</sup>; <sup>1</sup>Purdue University, Department of Chemistry, West Lafayette, IN; <sup>2</sup>Purdue University Department of Chemistry, West Lafayette, IN
- MP 362 **Mass Spectrometry Imaging Analysis Reveals Dysregulated Metabolic Pathways in an Inherited Form of Kidney Disease;** Ian Tamayo<sup>1</sup>; Mengyuan Ge<sup>2</sup>; Alessia Fornoni<sup>2</sup>; Kumar Sharma<sup>1</sup>; <sup>1</sup>UT Health San Antonio, San Antonio, TX; <sup>2</sup>University of Miami, Miami, FL
- MP 363 **Multiplex and multiomic MS imaging of drugs, metabolites, and immunolabeled pathogenic protein markers within a single tissue section;** Prem Shankar<sup>1</sup>; Reina N. Paez<sup>1</sup>; David Beaver<sup>1</sup>; Bandana Bera<sup>1</sup>; Brendan Prideaux<sup>1</sup>; <sup>1</sup>University of Texas Medical Branch, Galveston, TX

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- MP 364 **Mass spectrometry imaging with spatially resolved omics in mouse brain;** Saira Hameed<sup>1</sup>; Matija Lagator<sup>2</sup>; Daniel Simon<sup>1, 3</sup>; Kenny Robinson<sup>1</sup>; Felicia Green<sup>1</sup>; Bela Paizs<sup>1</sup>; Zoltan Takats<sup>1, 3</sup>; <sup>1</sup>Rosalind Franklin Institute, Didcot, United Kingdom; <sup>2</sup>Rosalind Franklin Institute, Harwell, United Kingdom; <sup>3</sup>Imperial College London, Hammersmith Hospital, London, United Kingdom
- MP 365 **A comprehensive view of molecular and cellular heterogeneity in S. aureus-infected tissue microenvironments;** Jacqueline M. Van Ardenne<sup>1, 2</sup>; Lukasz Migas<sup>2, 3</sup>; Morad C. Malek<sup>2, 4</sup>; Roy Lardenoije<sup>5</sup>; Jeffrey A. Freiberg<sup>6, 7</sup>; Kyle T. Enriquez<sup>7, 8, 9</sup>; Katherine N. Gibson-Corley<sup>9</sup>; Angela R. S. Kruse<sup>2, 4</sup>; Melissa A. Farrow<sup>2, 10</sup>; Joana P. Gonçalves<sup>5</sup>; Raf Van De Plas<sup>2, 3, 10</sup>; Eric P. Skaar<sup>7, 9, 11</sup>; Jeffrey M. Spraggins<sup>1, 2, 4, 9, 10</sup>; <sup>1</sup>Department of Chemistry, Vanderbilt University, Nashville, TN; <sup>2</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>3</sup>Delft Center for Systems and Control, Delft University of

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- Technology, Delft, Netherlands; <sup>4</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>5</sup>Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands; <sup>6</sup>Division of Infectious Diseases, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; <sup>7</sup>Vanderbilt Institute for Infection, Immunology and Inflammation, Vanderbilt University Medical Center, Nashville, TN; <sup>8</sup>Vanderbilt University Medical Scientist Training Program, Vanderbilt University School of Medicine, Nashville, TN; <sup>9</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; <sup>10</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>11</sup>Vanderbilt Institute for Chemical Biology, Vanderbilt University, Nashville, TN
- MP 366 **Selective Mapping of Lipids in the Brain using Desorption Electrospray Ionization Coupled with Multiple Reaction Monitoring Tandem Mass Spectrometry**; Marios Georgiadis<sup>1</sup>; Michael Zeineh<sup>1</sup>; Inma Cobos<sup>2</sup>; Jeffrey Nirschl<sup>2</sup>; Xiaowei Vivian Lu<sup>3</sup>; Ryan Leib<sup>3</sup>; Allis Chien<sup>3</sup>; Andrew Baker<sup>4</sup>; <sup>1</sup>Department of Radiology, Stanford School of Medicine, Stanford, CA; <sup>2</sup>Department of Pathology, Stanford School of Medicine, Stanford, CA; <sup>3</sup>Stanford University Mass Spectrometry, Stanford, California; <sup>4</sup>Waters Corporation, Pleasanton, CA
- MP 367 **A spatial multiomics workflow on a new benchtop MALDI-TOF instrument for deciphering the lipid and expressed protein landscape in tissues**; Janina Oetjen<sup>1</sup>; Corinna Henkel<sup>1</sup>; Ulrike Schweiger Hufnagel<sup>1</sup>; Tobias Boskamp<sup>1</sup>; Sebastian Boehm<sup>1</sup>; Christoph Nordmann<sup>1</sup>; Andree Schuster<sup>1</sup>; Katherine Stumpo<sup>2</sup>; Michael Easterling<sup>2</sup>; Jens Christmann<sup>3</sup>; Andrea Tannapfel<sup>3</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; <sup>2</sup>Bruker Scientific, 40 Manning Road, Billerica, MA; <sup>3</sup>Institute for Pathology, Ruhr-University Bochum, Bürkle-de-la-Camp-Platz 1, 44789 Bochum, Germany
- MP 368 **Imaging Mass Spectrometry Reveals Spatially-Resolved Biomolecular Response to Heavy Metal Intoxication**; Emilio S Rivera<sup>1, 2</sup>; Kes A. Luchini<sup>1, 2</sup>; Tara Harvey<sup>1, 2</sup>; Madison Grace Thornhill<sup>1, 2</sup>; Robert M. Taylor<sup>3</sup>; Abdul-Mehdi S. Ali<sup>3</sup>; Alicia M. Bolt<sup>4</sup>; Srinu R. Gadam<sup>3</sup>; Abigale S Mikolitis<sup>1, 2</sup>; Zachary J. Sasiene<sup>1, 2</sup>; Joshua D. Breidenbach<sup>1, 2</sup>; Ethan M. McBride<sup>1, 2</sup>; Brett R. Blackwell<sup>1, 2</sup>; Austin R. Anderson<sup>1, 2</sup>; Lauren K. Heine<sup>1, 2</sup>; Chi-Yen Tseng<sup>1, 2</sup>; Jessica A. Salguero<sup>1, 2</sup>; Francisca E. Rodriguez<sup>1, 2</sup>; Salvator J. Palmisano<sup>1, 2</sup>; Erick S. LeBrun<sup>1, 2</sup>; Phillip M. Mach<sup>1, 2</sup>; Justin T. Baca<sup>3</sup>; Trevor G. Glaros<sup>1, 2</sup>; <sup>1</sup>Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>3</sup>Department of Emergency Medicine, University of New Mexico School of Medicine, Albuquerque, NM; <sup>4</sup>Department of Pharmaceutical Sciences, College of Pharmacy, University of New Mexico, Albuquerque, NM
- MP 369 **Spatially resolved single-cell multi-omics via integration of metabolome and proteome profiling with mass spectrometry imaging**; Hua Zhang<sup>1</sup>; Xudong Shi<sup>2</sup>; Kelly H. Lu<sup>3</sup>; Zicong Wang<sup>1</sup>; Haiyan Lu<sup>1</sup>; Yuan Liu<sup>1</sup>; Nathan V. Welham<sup>2</sup>; Lingjun Li<sup>1, 3</sup>; <sup>1</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Surgery, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- MP 370 **Unveiling Spatial Metabolism in Mammalian Organ tissues: A Knowledge Base with Multimodal approach**; Prasad Phapale<sup>1</sup>; Siva Swapna Kasarla<sup>1</sup>; Karl Smith<sup>1</sup>; Antonia Fecke<sup>1</sup>; <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., Dortmund, Germany
- MP 371 **In-Depth Mapping of Antibodies and the Proteome by A New Generation of Micro-Scaffold-Assisted Proteomics (MASP) with Higher Spatial Resolution**; Shihan Huo<sup>1</sup>; Min Ma<sup>1</sup>; Shuo Qian<sup>1</sup>; Ming Zhang<sup>1</sup>; Jie Pu<sup>1</sup>; Xiaoyu Zhu<sup>1</sup>; Sailee Rasam<sup>1</sup>; Jun Qu<sup>1</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY
- MP 372 **Quantitatively Mapping Thousands of Phosphorylated Proteins at the Whole Tissue Level by Micro-Scaffold-Assisted Spatial Phosphoproteomics (MASPHOS)**; Min Ma<sup>1</sup>; Shihan Huo<sup>1</sup>; Ming Zhang<sup>1</sup>; Shuo Qian<sup>1</sup>; Maosheng Wei<sup>1</sup>; Jun Qu<sup>1</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY
- MP 373 **Spatial Metabolomics and Isotope Tracing Reveal Division of Labor in the Mammalian Liver and Intestine**; Laith Samarah<sup>1</sup>; Xi Xing<sup>1</sup>; Clover Zheng<sup>1</sup>; Amichay Afriat<sup>1</sup>; Cong Ma<sup>1</sup>; Michael MacArthur<sup>1</sup>; Connor Jankowski<sup>1</sup>; Benjamin J. Raphael<sup>1</sup>; Joshua D. Rabinowitz<sup>1</sup>; <sup>1</sup>Princeton University, Princeton, NJ
- MP 374 **Revealing the Molecular Underpinnings of Islet Dysfunction with Integrated Imaging Mass Spectrometry and Spatial Transcriptomics**; Angela R. S. Kruse<sup>1, 5</sup>; Kristie I. Aamodt<sup>2</sup>; Chunhua Dai<sup>3</sup>; Morad C Malek<sup>4, 5</sup>; Roy Lardenoije<sup>6</sup>; Lukasz Migas<sup>7</sup>; Melissa A. Farrow<sup>4, 5</sup>; Diane Saunders<sup>3</sup>; Richard M. Caprioli<sup>4, 8, 9</sup>; Raf Van De Plas<sup>7, 10</sup>; Joana P. Gonçalves<sup>6</sup>; Alvin C. Powers<sup>2, 3, 11</sup>; Jeffrey M Spraggins<sup>4, 5, 8, 9, 12</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Department of Molecular Physiology and Biophysics, Vanderbilt University School of Medicine, Nashville, TN; <sup>3</sup>Division of Diabetes, Endocrinology and Metabolism, Vanderbilt University Medical Center, Nashville, TN; <sup>4</sup>Mass Spectrometry Research Center, Nashville, TN; <sup>5</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>6</sup>Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands; <sup>7</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>8</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>9</sup>Department of Chemistry, Vanderbilt University, Nashville, TN; <sup>10</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>11</sup>Veteran Affairs Tennessee Valley Healthcare System, Nashville, TN; <sup>12</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN
- MP 375 **Single-voxel proteomics for 2D-proteome mapping human spleen and mouse brain tissues**; Zhangyang Xu<sup>1</sup>; Reta Birhanu Kitata<sup>1</sup>; Rosalie K. Chu<sup>2</sup>; Rui Zhao<sup>2</sup>; Daniel J. Orton<sup>2</sup>; Thomas L. Fillmore<sup>2</sup>; Matthew J. Gaffrey<sup>1</sup>; Tong Zhang<sup>1</sup>; Tao Liu<sup>1</sup>; Clive H. Wasserfall<sup>3</sup>; Song-Lin Ding<sup>4</sup>; Tujin Shi<sup>1</sup>; <sup>1</sup>Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington; <sup>2</sup>Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; <sup>3</sup>Department of Pathology, Immunology, and Laboratory Medicine, Diabetes Institute, College of Medicine, University of Florida, Gainesville, Florida; <sup>4</sup>Allen Institute for Brain Science, Seattle, Washington
- MP 376 **Preserving RNA integrity after Imaging Mass Spectrometry for Integrated Spatial Transcriptomics on Single Tissue Sections**; Morad C Malek<sup>1, 2</sup>; Martin Dufresne<sup>1, 3</sup>; Roy Lardenoije<sup>4</sup>; Angela RS Kruse<sup>2, 5</sup>; Lukasz Migas<sup>1, 6</sup>; Melissa A. Farrow<sup>1, 3</sup>; Katerina V Djambazova<sup>1, 2</sup>; Raf Van De Plas<sup>1, 3, 6</sup>; Joana P Gonçalves<sup>4</sup>; Jeffrey M Spraggins<sup>1, 2, 3, 7, 8</sup>; <sup>1</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>2</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>3</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>4</sup>Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands; <sup>5</sup>Mass Spectrometry Research Center, Nashville, TN; <sup>6</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>7</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; <sup>8</sup>Department of Chemistry, Vanderbilt University, Nashville, TN
- MP 377 **Laser Ablation Sampling and MALDI Imaging for Tissue Lipidomics**; Kadeem O Hayes<sup>1</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA

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- MP 378 **Constructing a Foundational Molecular Atlas of the Normal Human Kidney with Multimodal Molecular Imaging;** Olof Gerdur Isberg<sup>1, 2</sup>; Lukasz Migas<sup>3</sup>; Melissa A. Farrow<sup>1, 4, 5</sup>; Jamie L. Allen<sup>1, 4</sup>; Felipe A. Moser<sup>3</sup>; Léonore E.M. Tideman<sup>3</sup>; Angela R. S. Kruse<sup>1, 2</sup>; Ellie L. Pingry<sup>1, 2</sup>; Morad C. Malek<sup>1</sup>; Thai H. Pham<sup>1, 2</sup>; Madeline E. Colley<sup>1, 4</sup>; Haichun Yang<sup>5, 6</sup>; Mark P. DeCaestecker<sup>2, 7</sup>; Agnes B. Fogo<sup>5, 6, 7</sup>; Joana Goncalves<sup>8</sup>; Raf Van De Plas<sup>3</sup>; Jeffrey M. Spraggins<sup>1, 2, 4, 5</sup>; <sup>1</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>2</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>3</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>4</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>5</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; <sup>6</sup>Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; <sup>7</sup>Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; <sup>8</sup>Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands
- MP 379 **Organoid analysis using ultra-high lateral resolution AP-SMALDI mass spectrometry imaging;** Parviz Ghezellou<sup>1</sup>; Elisa Badin<sup>1</sup>; Max A. Müller<sup>1, 2</sup>; Svenja Pauer<sup>1</sup>; Jasmin Ballout<sup>1</sup>; Vinicius Pinho Dos Reis<sup>3</sup>; Eva Hecker<sup>3</sup>; Martin Diener<sup>1</sup>; Kerstin Strupat<sup>4</sup>; Bernhard Spengler<sup>1</sup>; <sup>1</sup>Justus Liebig University, Giessen, Germany; <sup>2</sup>Transmit GmbH, Giessen, Germany; <sup>3</sup>Philipps University, Marburg, Germany; <sup>4</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- MP 380 **Single cell multi-omic mass spectrometry imaging for the human bone marrow microenvironment;** Patricia Favaro<sup>1</sup>; Davide Franchina<sup>1</sup>; Ke Xuan Leow<sup>1</sup>; Daniel Ho<sup>1</sup>; Trevor Bruce<sup>1</sup>; Xiaowei Lu<sup>1</sup>; Marc Bosse<sup>1</sup>; Richard R Drake<sup>2</sup>; Albert Tsai<sup>1</sup>; Michael Angelo<sup>1</sup>; Sean Bendall<sup>1</sup>; <sup>1</sup>Stanford University, Stanford, CA; <sup>2</sup>Medical University of South Carolina, Charleston, SC
- MP 381 **SPOT: Spatial Proteomics through On-site Tissue-protein-labeling;** Yuanwei Xu<sup>1, 2</sup>; T.Mamie Lih<sup>2</sup>; Angelo Michael De Marzo<sup>2, 3</sup>; Qing Kay Lj<sup>3, 4</sup>; Hui Zhang<sup>1, 2, 3</sup>; <sup>1</sup>Johns Hopkins University, Baltimore; <sup>2</sup>Johns Hopkins University School of Medicine, Baltimore city, MD; <sup>3</sup>Johns Hopkins Sidney Kimmel Comprehensive Cancer Center, Baltimore, MD; <sup>4</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- MP 382 **Delineating AβPlaque Associated Lipid Co-Aggregation Dynamics Using Pulse-Chase Spatial Multiomics;** Junyue Ge<sup>1</sup>; Durga Jha<sup>1</sup>; Srinivas Koutarapu<sup>1</sup>; Maciej Dulewicz<sup>1</sup>; Henrik Zetterberg<sup>1, 2, 3, 4, 5</sup>; Kaj Blennow<sup>1, 2</sup>; Jörg Hanrieder<sup>1, 2, 3</sup>; <sup>1</sup>University of Gothenburg, Gothenburg, Sweden; <sup>2</sup>Sahlgrenska University Hospital, Gothenburg, Sweden; <sup>3</sup>University College London, London, United Kingdom; <sup>4</sup>Hong Kong Center for Neurodegenerative Diseases, Hong Kong, China; <sup>5</sup>University of Wisconsin-Madison, Madison, WI
- MP 383 **Rapid QCL-based Mid-Infrared Vibrational Microscopy guides Deep Magnetic Resonance MALDI MSI;** Stefan Schmidt<sup>1</sup>; Lars Gruber<sup>2, 3</sup>; Thomas Enzlein<sup>2</sup>; Huong Giang Vo<sup>4</sup>; James Lucas Cairns<sup>2</sup>; Denis Abu Sammour<sup>2</sup>; Matthias Eckhardt<sup>5</sup>; Laura Bindila<sup>4</sup>; Carsten Hopf<sup>2, 3</sup>; <sup>1</sup>Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), University of Applied Sciences Mannheim, Mannheim, Germany; <sup>2</sup>Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), University of Applied Sciences Mannheim, Mannheim, Germany; <sup>3</sup>Medical Faculty, Heidelberg University, Heidelberg, Germany; <sup>4</sup>Clinical Lipidomics Unit, Institute of Physiological Chemistry, University of Medical Center of the JGU Uni Mainz, Mainz, Germany; <sup>5</sup>Institute of Biochemistry and Molecular Biology, University of Bonn, Bonn, Germany, Bonn, Germany
- MP 384 **How Clean is “Clean”? Going Above and Beyond the Conventional Check-Clean with a Rapid, DART-MS Protocol;** William L Fatigante; *Bruker Applied Mass Spectrometry, Billerica, MA*
- MP 385 **Trace-Level Quantification of N-Nitrosomethylpropylamine Impurity by LC-HRMS;** Ziyu Wang<sup>1</sup>; Holly M. Shackman<sup>1</sup>; Sloan Ayers<sup>1</sup>; Michael B. Peddicord<sup>1</sup>; Scott A. Miller<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb, New Brunswick, NJ
- MP 386 **Automated Sample Preparation using PAL3 RTC System for EPA 8270E Semi-volatile Organic Analysis by GC/TQ;** Tarun Anumol<sup>1</sup>; Gwen Sin Yee Lim<sup>2</sup>; Aimei Zou<sup>3</sup>; <sup>1</sup>Agilent Technologies, Wilmington, DE; <sup>2</sup>CTC Analytics AG, Zwingen, Switzerland; <sup>3</sup>Agilent Technologies Singapore, Singapore, Singapore
- MP 387 **Automated Sample Preparation and Analysis of Organochlorine Pesticides (OCP's) in Drinking Water;** Callum Morgan<sup>1</sup>; Bryan White<sup>2</sup>; Joel Ferrer<sup>3</sup>; Aaron Boice<sup>3</sup>; Anastasia Andrianova<sup>4</sup>; <sup>1</sup>Agilent Technologies UK Limited, Cheadle, United Kingdom; <sup>2</sup>Agilent Technologies LDA UK Ltd, Didcot, United Kingdom; <sup>3</sup>Agilent Technologies, Santa Clara, CA; <sup>4</sup>Agilent Technologies, Wilmington, DE
- MP 388 **Implementation of a digital quality management system for enhanced mass spectrometry practices in a large-scale proteomics laboratory;** Casey W Coutelin Johnson<sup>1</sup>; Shruti Rao<sup>1</sup>; Salomen Ashaq<sup>1</sup>; Susan M. Mockus<sup>1</sup>; <sup>1</sup>Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA
- MP 389 **High resolution process gas monitoring by infITOF to shed light on the growth process of β-Ga2O3 by MOVPE;** Yoshihiko Takinami<sup>1</sup>; Kazutaka Ikenaga<sup>2</sup>; Takahito Okuyama<sup>3</sup>; Shogo Sasaki<sup>3</sup>; Masato Ishikawa<sup>4</sup>; Yoshinao Kumagai<sup>3</sup>; <sup>1</sup>Kanomax Analytical, Incorporated, Chofu, Japan; <sup>2</sup>Taiyo Nippon Sanso Corporation, Minato-ku, Japan; <sup>3</sup>Tokyo University of Agriculture and Technology, Koganei-shi, Japan; <sup>4</sup>Gas-Phase Growth Ltd., Koganei-shi, Japan
- MP 390 **Automated sample preparation instrument for large-scale proteomics pre-processing;** Lin He<sup>1</sup>; Yan Zhao<sup>1</sup>; Weij Sun<sup>1</sup>; Longqin Sun<sup>1</sup>; <sup>1</sup>Beijing Qinglian Biotech Co., Ltd, Beijing, China
- MP 391 **Developing a Contaminant Spot Check and Removal Assay (ContamSPOT) for Mass Spectrometry Analysis;** Noah Smeriglio<sup>1</sup>; Haorong Li<sup>1</sup>; Wan Nur Atiqah Binti Mazli<sup>1</sup>; Katharine Bendel<sup>1</sup>; Ling Hao<sup>1</sup>; <sup>1</sup>George Washington University, Washington D.C., DC
- MP 392 **High-speed compound quality assessment using Acoustic Ejection Mass Spectrometry;** Anuja Bhalkikar<sup>1</sup>; Aaron Stella<sup>2</sup>; Jacob Watson McCabe<sup>2</sup>; Han Joo Lee<sup>2</sup>; <sup>1</sup>Sciex, Framingham; <sup>2</sup>SCIEX, USA, Framingham, MASSACHUSETTS
- MP 393 **Stability Testing of Consumer Drug Products for Benzene in Real-Time using SIFT-MS;** David Light<sup>1</sup>; Nicola Zenzola<sup>1</sup>; Amber Hudspeth<sup>1</sup>; Mara Dubnicka<sup>1</sup>; Kaury Kucera<sup>1</sup>; Wolfgang Hinz<sup>1</sup>; Christopher Bunick<sup>2</sup>; Arash Dabestani<sup>3</sup>; Leslie P. Silva<sup>4</sup>; <sup>1</sup>Valisure, LLC, New Haven, CT; <sup>2</sup>Yale University, West Haven, CT; <sup>3</sup>Long Island University, Brooklyn, NY; <sup>4</sup>Syft Technologies, Anaheim, CA

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- MP 394 **Prioritizing Biotransformations in LC-MS/MS-based non-targeted Metabolomics with ChemProp2;** Abzer K Pakkiri Shah<sup>1</sup>; Paolo Stincone<sup>1, 2</sup>; Anne Grieshammer<sup>1, 3</sup>; Axel Walter<sup>1, 4</sup>; Simon B Knoblauch<sup>2</sup>; Giovanni Andrea Vitale<sup>1</sup>; Mingxun Wang<sup>5</sup>; Lisa Maier<sup>1, 3</sup>; Daniel Petras<sup>1, 6</sup>; <sup>1</sup>University of Tuebingen, CMFI Cluster of Excellence, Interfaculty Institute of Microbiology and Infection Medicine, Tübingen, Germany; <sup>2</sup>University of Tuebingen, Center for Plant Molecular Biology, Tübingen, Germany; <sup>3</sup>Cluster of Excellence EXC 2124 Controlling Microbes to Fight Infections, University of Tübingen, Tübingen, Germany; <sup>4</sup>Applied Bioinformatics, Department of Computer Science, University of Tübingen, Tübingen, Germany; <sup>5</sup>University of

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- California Riverside, Department of Computer Science, Riverside, CA; <sup>6</sup>University of California Riverside, Department of Biochemistry, Riverside, CA
- MP 395 **Metabolomics: Mapping Evolution and Trends in the Field with AI Tools**; Olatomiwa O Bifarin<sup>1</sup>; Varun S Yelluru<sup>2</sup>; Facundo M. Fernandez<sup>1, 3</sup>; <sup>1</sup>School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>School of Computer Science, Georgia Institute of Technology, Atlanta, GA; <sup>3</sup>Petit Institute of Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA
- MP 396 **MyCompoundID 2.0: An Evidence-Based Metabolome Library for Metabolite Identification**; Bowen Yang<sup>1</sup>; Hao Li<sup>1</sup>; Shuang Zhao<sup>2</sup>; Liang Li<sup>1, 2</sup>; <sup>1</sup>University of Alberta, Edmonton, AB; <sup>2</sup>The Metabolomics Innovation Centre (TMIC), Edmonton, AB
- MP 397 **Flora: Learning fragmentation patterns of small compounds with graph neural networks**; Yanek Nowatzky<sup>1</sup>; Thilo Muth<sup>2</sup>; Philipp Benner<sup>1</sup>; <sup>1</sup>Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany; <sup>2</sup>Robert Koch Institute, Berlin, Germany
- MP 398 **Big-data metabolomics: annotating MS/MS spectra for structures and biological relevance by querying extremely large scale datasets**; Yuanyue Li<sup>1</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA
- MP 399 **Unmasking lipid double bond positions in routine LC-MS/MS data**; Leonida M Lamp<sup>1</sup>; Joseph P Argus<sup>2</sup>; Aaron M Armando<sup>2</sup>; Gosia M Murawska<sup>2</sup>; Oswald Quehenberger<sup>2</sup>; Edward A Dennis<sup>2</sup>; Jürgen Hartler<sup>1, 3</sup>; <sup>1</sup>Pharmaceutical Sciences, University of Graz, Graz, Austria; <sup>2</sup>Department of Pharmacology, University of California San Diego, La Jolla, CA; <sup>3</sup>Field of Excellence BioHealth, University of Graz, Graz, Austria
- MP 400 **AI-driven peak picking and integration using chromatograms and deep neural networks**; Daniel Pelisek<sup>1</sup>; Radu Talmazan<sup>1</sup>; Martin Buratti<sup>1</sup>; Tuan Hai Pham<sup>1</sup>; Alice Limonciel<sup>1</sup>; <sup>1</sup>biocrates life sciences ag – Eduard-Bodem-Gasse 8, Innsbruck, Austria
- MP 401 **Enhanced Structural Modification Site Localization through MS/MS Spectral Alignment and Molecular Network Refinement**; Mohammad Reza Zare Shahneh<sup>1</sup>; Michael Strobel<sup>1</sup>; Giovanni Andrea Vitale<sup>2</sup>; Christian Geibel<sup>2</sup>; Vanessa V Phelan<sup>3</sup>; Daniel Petras<sup>4</sup>; Allegra T Aron<sup>5</sup>; Yasin El Abiead<sup>6</sup>; Neha Garg<sup>7</sup>; Mingxun Wang<sup>1</sup>; <sup>1</sup>University of California Riverside, Department of Computer Science, Riverside, CA; <sup>2</sup>University of Tuebingen, Interfaculty Institute of Microbiology and Infection Medicine, Tuebingen, Germany; <sup>3</sup>University of Colorado, Anschutz Medical Campus, Department of Pharmaceutical Sciences, Aurora, CO; <sup>4</sup>University of California Riverside, Department of Biochemistry, Riverside, CA; <sup>5</sup>University of Denver, Denver, CO; <sup>6</sup>University of California San Diego, La Jolla, CA; <sup>7</sup>Georgia Institute of Technology, Atlanta, GA
- MP 402 **TIMS-enabled 4D-Metabolomics workflow for the automated analysis of derivatised analytes**; Jesper Havelund<sup>1</sup>; Aiko Barsch<sup>2</sup>; Sofie Weinkouff<sup>2</sup>; Nikolas Kessler<sup>2</sup>; Heiko Neuweger<sup>2</sup>; Matthew R Lewis<sup>2</sup>; Nils J. Færgeman<sup>1</sup>; Ryo Nakabayashi<sup>3</sup>; <sup>1</sup>Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark; <sup>2</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; <sup>3</sup>Bruker Japan K.K., Yokohama, Japan
- MP 403 **Mapping of electron impact ionization time-of-flight and chemical ionization Fourier transform gas chromatographic mass spectrometry data by Genedata Expressionist**; Josh Prybil<sup>1</sup>; Joseph P. Shambaugh<sup>2</sup>; John D. Everard<sup>1</sup>; Brian M. Ruddy<sup>1</sup>; <sup>1</sup>Corteva Agriscience, Johnston, IA; <sup>2</sup>Genedata Inc., Lexington, Massachusetts
- MP 404 **Automated LC-MS/MS Glycomic Structural Feature Annotation**; Xavier A. Holmes<sup>1</sup>; Armin Oulomi<sup>1</sup>; Michael Russelle S. Alvarez<sup>1</sup>; Ryan Schindler<sup>1</sup>; Tristan Seales<sup>1</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>University of California Davis, Davis, CA
- MP 405 **Utilizing Skyline in Automated System Suitability Testing, Data QC, and Metabolite Quantification for Microchip CE-MS Analysis**; Sam Stewart<sup>1</sup>; Erin A. Redman<sup>2</sup>; Joshua P. Guerrette<sup>2</sup>; Nicholas Shulman<sup>3</sup>; Brian S Pratt<sup>3</sup>; Michael J. MacCoss<sup>3</sup>; Brendan MacLean<sup>3</sup>; J. Will Thompson<sup>2</sup>; <sup>1</sup>908 Devices Inc., Boston, MA; <sup>2</sup>908 Devices Inc, Morrisville, NC; <sup>3</sup>University of Washington - Genome Sciences, Seattle, WA
- MP 406 **PAMDA: Publicly Available Metabolomics Dataset Alignment and Analysis of Human Urine Measured by RPLC-MS**; Hani Habra<sup>1</sup>; Yamil Simon<sup>1</sup>; Tytus Mak<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD
- MP 407 **LipidTarget: An Integrated Platform for Targeted HPLC-MSn Characterization and Quantification of Lipid sn-Positional Isomers**; Hongyuan Yang<sup>1</sup>; Tingyuan Yang<sup>1</sup>; Jiaxin Feng<sup>1</sup>; Xin Yan<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX
- MP 408 **Metabolite-specific inter-individual variability: A meta-analysis of metabolomics datasets and the need for log transformation**; Aviral Singh<sup>1</sup>; Renu Pandey<sup>2</sup>; Gauri Desai<sup>2</sup>; Prajval Nakarni<sup>1</sup>; Vivek Mishra<sup>1</sup>; Deepti Sahasrabudhe<sup>2</sup>; Pramod Wangikar<sup>1, 2</sup>; <sup>1</sup>Clarity Bio Systems India Pvt. Ltd., Pune, India; <sup>2</sup>Indian Institute of Technology Bombay, Mumbai, India
- MP 409 **Comprehensive structural annotation of polar metabolites in human plasma using unified-HILIC/AEX retention time prediction and HRMS/MS substructure information**; Taihei Torigoe<sup>1</sup>; Masatomo Takahashi<sup>1</sup>; Omidreza Heravizadeh<sup>2</sup>; Kazuki Ikeda<sup>1</sup>; Kohta Nakatani<sup>1</sup>; Takeshi Bamba<sup>1</sup>; Yoshihiro Izumi<sup>1</sup>; <sup>1</sup>Medical Institute of Bioregulation, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka-shi, Japan; <sup>2</sup>Graduate School of Systems Life Sciences, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka-shi, Japan
- MP 410 **Lipidex 2 integrates MSn tree-based fragmentation methods and quality control modules to improve discovery lipidomics**; Benton J. Anderson<sup>1, 2</sup>; Dain R. Brademan<sup>3</sup>; Yuchen He<sup>3</sup>; Corinne E. Moss<sup>1</sup>; Katherine A. Overmyer<sup>1, 2, 3</sup>; Gwendalyn J. Randolph<sup>5</sup>; Joshua J. Coon<sup>1, 2, 3, 6</sup>; <sup>1</sup>Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI; <sup>3</sup>Morgridge Institute for Research, Madison, WI; <sup>4</sup>Department of Biophysics, University of Wisconsin-Madison, Madison, WI; <sup>5</sup>Department of Pathology and Immunology, Washington University School of Medicine, St. Louis, MO; <sup>6</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- MP 411 **Enhanced Spectrum Clustering For Increased Interpretability of Molecular Networking**; Janne Heirman<sup>1</sup>; Wout Bittremieux<sup>1</sup>; <sup>1</sup>University of Antwerp, Antwerpen, Belgium
- MP 412 **Chemical Annotation Propagation for Molecular Networks**; Bela Paizs<sup>1, 2</sup>; Logan Mackay<sup>1</sup>; Amar Rai<sup>3</sup>; Anthony J Devlin<sup>1</sup>; Zoltan Takats<sup>2, 3</sup>; <sup>1</sup>Rosalind Franklin Institute, Didcot, United Kingdom; <sup>2</sup>deShape Ltd., London, United Kingdom; <sup>3</sup>Imperial College London, London, United Kingdom
- MP 413 **MS2LIPID: lipid subclass prediction using tandem mass spectral data**; Nami Sakamoto<sup>1</sup>; Takaki Oka<sup>1</sup>; Yuki Matsuzawa<sup>1</sup>; Kozo Nishida<sup>1</sup>; Aya Hori<sup>2</sup>; Makoto Arita<sup>2, 3, 4</sup>; Hiroshi Tsugawa<sup>1, 2, 4, 5, 6</sup>; <sup>1</sup>Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology, Koganei-shi, Japan; <sup>2</sup>Laboratory for Metabolomics, RIKEN Center for Integrative Medical Sciences, Yokohama, Japan; <sup>3</sup>Keio University, Graduate School of Pharmaceutical Sciences, Division of Physiological Chemistry and Metabolism, Minato-ku, Japan; <sup>4</sup>Molecular and Cellular Epigenetics Laboratory, Graduate School of Medical Life Science, Yokohama City University, Yokohama, Japan; <sup>5</sup>RIKEN Center for Brain Science, Wako, Japan; <sup>6</sup>RIKEN Center for Sustainable Resource Science, Yokohama, Japan



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- MP 414 **Deep Learning for Small Molecule Analog Discovery From Untargeted Mass Spectrometry**; Juan Sebastian Piedrahita Giraldo<sup>1</sup>; Thomas De Vijlder<sup>2</sup>; Kris Laukens<sup>1</sup>; Wout Bittremieux<sup>1</sup>; <sup>1</sup>University of Antwerp, Antwerp, Belgium; <sup>2</sup>Janssen Pharmaceutica NV, Beerse, Belgium
- MP 415 **Evaluation of an R-based metabolomics data processing workflow against a novel benchmark metabolomics dataset**; Corey D Broeckling<sup>1</sup>; Linxing Yao<sup>1</sup>; Nathan Montgomery<sup>1</sup>; Kevin Y Cho<sup>2</sup>; Gary J. Patti<sup>2</sup>; Xiuxia Du<sup>3</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO; <sup>2</sup>Washington University in Saint Louis, St. Louis, MO; <sup>3</sup>University of North Carolina at Charlotte, Charlotte, NC
- MP 416 **Deciphering the Interplay between 16S rRNA-seq and Metabolome through Weighted Correlation Network Analysis**; Minsoo Son<sup>1</sup>; Jong Hee Song<sup>1</sup>; Young Ah Goo<sup>1</sup>; <sup>1</sup>MTAC, MGI, Washington University School of Medicine in Saint Louis, Saint Louis, MO
- MP 417 **Reanalysis of public domain, untargeted metabolomics datasets using AI-powered workflow: Unraveling novel biomarkers for severe COVID**; Prajval Nakrani<sup>1</sup>; Nived Krishnan Santhosh<sup>1</sup>; Aviral Singh<sup>1</sup>; Vivek Mishra<sup>1</sup>; Sachin Patil<sup>1</sup>; Pramod P Wangikar<sup>1,2</sup>; <sup>1</sup>Clarity Bio Systems India Pvt. Ltd., Pune, India; <sup>2</sup>Indian Institute of Technology Bombay, Mumbai, India
- MP 418 **Conversion and integration of OMICS data from a prototype, benchtop multi-reflecting time-of-flight (MRT) platform with third-party informatic workflows**; Lee A Gethings<sup>1</sup>; Ian Morns<sup>1</sup>; Pete Reay<sup>1</sup>; Simon Jones<sup>1</sup>; Nyasha Munjoma<sup>1</sup>; Jayne Kirk<sup>1</sup>; Richard Lock<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom
- MP 419 **Extensive multi language API-support and novel annotation features in SIRIUS**; Markus Fleischauer<sup>1</sup>; Kai Dührkop<sup>1</sup>; Martin A. Hoffmann<sup>2</sup>; Marcus Ludwig<sup>2</sup>; Nils A. Haupt<sup>1</sup>; Martin Engler-Lukajewski<sup>2</sup>; Jonas Emmert<sup>1,3</sup>; Michael Stravs<sup>4</sup>; Sebastian Böcker<sup>1</sup>; <sup>1</sup>Friedrich Schiller University Jena, Jena, Germany; <sup>2</sup>Bright Giant GmbH, Jena, Germany; <sup>3</sup>International Max Planck Research School "Chemical Communication in Ecological Systems", Max Planck Institute for Chemical Ecology, Jena, Germany; <sup>4</sup>Eawag (Swiss Federal Institute of Aquatic Science and Technology) / Environmental Microbiology, Dübendorf, Switzerland
- MP 420 **Rapid and Precise Small Molecule Detection in Untargeted Metabolomics Using MetaboSLASH**; Suijun Li<sup>1,2</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>GlycoMS LLC, Bloomington, IN
- MP 421 **Isocitrate dehydrogenase 1 regulates cardiac metabolic adaptation during oncometabolic stress**; Kyoungmin Kim<sup>1</sup>; Brandon Faubert<sup>2</sup>; Yaqi Gao<sup>1</sup>; Lin Tan<sup>3</sup>; Nathaniel Snyder<sup>4</sup>; Philip L. Lorenzi<sup>5</sup>; Ralph DeBerardinis<sup>6</sup>; Anja Karlstaedt<sup>1</sup>; <sup>1</sup>Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA; <sup>2</sup>University of Chicago, Chicago, IL; <sup>3</sup>MD Anderson Cancer Center, Houston, Texas; <sup>4</sup>Temple University, Philadelphia, PA; <sup>5</sup>MD Anderson Cancer Center, Houston, TX; <sup>6</sup>UTSouthwestern Medical Center, Dallas, TX
- MP 422 **Learned representations from a transformer model trained on over 1 billion unannotated experimental spectra**; James Taylor<sup>1</sup>; Rose Lighthouse<sup>1</sup>; Christoph Krettlér<sup>1</sup>; Tyson Park<sup>1</sup>; Daniel Domingo-Fernandez<sup>1</sup>; David Healey<sup>1</sup>; <sup>1</sup>Enveda Biosciences, Boulder, CO
- MP 423 **Fast and Precise Hybrid Gas-Chromatography Mass-Spectrometry Metabolomics, Combining Single-Sample Targetted Search with Untargetted Composite Feature Detection**; Sami Teeny<sup>1</sup>; Dean P. Jones<sup>2</sup>; Young-Mi Go<sup>2</sup>; William Crandall<sup>2</sup>; Bill Liang<sup>2</sup>; Zackery Ryan Jarrell<sup>2</sup>; <sup>1</sup>University, Atlanta, GA; <sup>2</sup>Emory University, Atlanta, GA
- MP 424 **Machine learning based filtering improves untargeted lipid identification confidence**; Steven Tavis<sup>1,2</sup>; Matthew J. Keller<sup>2,3</sup>; Andrew Stai<sup>3</sup>; Diana Ramirez<sup>3</sup>; Frank Loeffler<sup>3</sup>; Robert L Hettich<sup>2</sup>; <sup>1</sup>University of Tennessee Knoxville, Knoxville, TN; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>3</sup>University of Tennessee, Knoxville, TN
- MP 425 **Lipidomic Characterization of Human Tonsillar B and T Cell Subsets by Matrix-Assisted Laser Desorption Ionization Time-Of-Flight Mass Spectrometry**; Jeferson A. Valencia-Dávila<sup>1</sup>; Benjamin L. Oyler<sup>1</sup>; Constantinos Petrovas<sup>3</sup>; Richard Koup<sup>1</sup>; <sup>1</sup>Tissue Analysis Core, Immunology Laboratory, Vaccine Research Center, NIAID, NIH, Bethesda, Maryland

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- MP 426 **Contrasting Trends: Increasing Variance at High Purity Levels in TMT Reporter Ion Analysis**; Eric Youngggon Kim<sup>1</sup>; Dhonggeon Won<sup>2</sup>; Chaewon Kang<sup>3</sup>; Hokeun Kim<sup>3</sup>; Sang-Won Lee<sup>3</sup>; Sangtae Kim<sup>1</sup>; <sup>1</sup>Bertis Bioscience, SAN DIEGO, CA; <sup>2</sup>Bertis Inc., Seoul, South Korea; <sup>3</sup>Department of Chemistry and Center for Proteogenome Research, Seoul, South Korea
- MP 427 **Phosphorylation site prediction model using structural context and its application to phosphopeptide identification**; Yujin Choo<sup>1</sup>; Seungjin Na<sup>2</sup>; Eunok Paek<sup>3,4,5</sup>; <sup>1</sup>Department of Artificial Intelligence, Hanyang University, Seoul, South Korea; <sup>2</sup>Korea Basic Science Institute, Cheongju, South Korea; <sup>3</sup>Department of Artificial Intelligence, Hanyang University, Seoul, South Korea; <sup>4</sup>Department of Computer Science, Hanyang University, Seoul, South Korea; <sup>5</sup>Institute of Artificial Intelligence Research, Hanyang University, Seoul, South Korea
- MP 428 **EndoGenius - An All-in-One Platform for Comprehensive Neuropeptide Characterization from DDA and DIA Datasets**; Lauren Fields<sup>1</sup>; Tina C Dang<sup>2</sup>; Mitchell Gray<sup>1</sup>; Wenxin Wu<sup>1</sup>; Angel E Ibarra<sup>1</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin; <sup>2</sup>University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin
- MP 429 **Prosit-PTM: Deep Learning Model Enhances Detection and Localization of Unseen PTMs**; Wassim Gabriel<sup>1</sup>; Vitor Sternlicht<sup>1</sup>; Daniel P. Zolg<sup>2</sup>; Polina Prokofeva<sup>2</sup>; Ludwig Lautenbacher<sup>1</sup>; Guillaume Médard<sup>2</sup>; Chien-Yun Lee<sup>3</sup>; Bernhard Kuster<sup>2</sup>; Mathias Wilhelm<sup>1</sup>; <sup>1</sup>Computational Mass Spectrometry, TUM, Freising, Germany; <sup>2</sup>Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; <sup>3</sup>Young Investigator Group: Mass Spectrometry in Systems Neurosciences, School of Life Sciences, Technical University of Munich, Freising, Germany
- MP 430 **ProteoBench: a community-curated platform for comparison of proteomics data analysis workflows**; Holda A Anagho<sup>1</sup>; Sven Degroevé<sup>2,3</sup>; Nadezhda T Doncheva<sup>1</sup>; Viktoria Dorfer<sup>4</sup>; Klemens Fröhlich<sup>5</sup>; Ralf Gabriels<sup>2,3</sup>; Vedran Kasalica<sup>6</sup>; Caroline Lennartsson<sup>1</sup>; Matthias Mattanovich<sup>7</sup>; Emmanuelle Mouton-Barbosa<sup>8</sup>; Martin Rykær<sup>1</sup>; Veit Schwämmle<sup>9</sup>; Maximilian T. Strauss<sup>1</sup>; Julian Uszkoreit<sup>10</sup>; Bart Van Puyvelde<sup>11</sup>; Tim Van Den Bossche<sup>2,3</sup>; Jakub Vašíček<sup>12,13</sup>; Henry Wobbel<sup>7</sup>; Witold Wolski<sup>14,15</sup>; Robbin Bouwmeester<sup>2,3</sup>; Marie Locard-Paulet<sup>8</sup>; <sup>1</sup>Novo Nordisk Foundation Center for Protein Research (CPR), University of Copenhagen, Copenhagen, Denmark; <sup>2</sup>VIB-Ugent Center for Medical Biotechnology, Gent, Belgium; <sup>3</sup>Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; <sup>4</sup>University of Applied Sciences Upper Austria, Hagenberg, Austria; <sup>5</sup>Proteomics Core Facility, Biozentrum Basel, University of Basel, Basel, Switzerland; <sup>6</sup>Netherlands eScience Center, Amsterdam, Netherlands; <sup>7</sup>Novo Nordisk Foundation Center for Basic Metabolic Research, Copenhagen, Denmark; <sup>8</sup>Institut de Pharmacologie et de Biologie Structurale (IPBS), Université de Toulouse, CNRS, Université Toulouse III - Paul Sabatier (UT3), Toulouse, France, Toulouse, France; <sup>9</sup>Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark; <sup>10</sup>Ruhr University Bochum, Medical Faculty, Medical Bioinformatics, Bochum, Germany; <sup>11</sup>ProGenTomics, Laboratory of Pharmaceutical Biotechnology, Ghent University, Ghent, Belgium; <sup>12</sup>Mohn Center for Diabetes Precision Medicine, Department of

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- Clinical Science, University of Bergen, Bergen, Norway; <sup>13</sup>Computational Biology Unit, Department of Informatics, University of Bergen, Bergen, Norway; <sup>14</sup>Functional Genomics Center Zurich – ETH Zurich/University of Zurich, Zurich, Switzerland; <sup>15</sup>Swiss Institute of Bioinformatics (SIB), Lausanne, Switzerland
- MP 431 **NeoFlow2: Enhancing Tumor-Specific HLA-I Peptide Identification by Integrating De Novo Sequencing and Customized Database Search in a Streamlined Proteogenomic Workflow;** Seunghyuk Choi<sup>1</sup>; Yongchao Dou<sup>1</sup>; Zhiao Shi<sup>1</sup>; Bing Zhang<sup>1</sup>; <sup>1</sup>Baylor College of Medicine, Houston, TX
- MP 432 **Alternating series approximation minimizes quantitative bias arising from incomplete isotope labeling;** Pin-Lian Jiang<sup>1</sup>; Louise Ulrich Kurt<sup>2</sup>; Isis Venturi Biembengut<sup>2</sup>; Fan Liu<sup>1</sup>; <sup>1</sup>Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; <sup>2</sup>Laboratory for Structural and Computational Proteomics, Fiocruz-Parana, Curitiba, Brazil
- MP 433 **Impact of the Peptide Identification Framework on the Results of Fast Photochemical Oxidation of Protein Analysis;** Marek Zakopcanik<sup>1,2</sup>; Daniel Kavan<sup>1</sup>; Petr Novak<sup>1</sup>; Dmitry S. Loginov<sup>1</sup>; <sup>1</sup>Institute of Microbiology, Praha - Vestec, Czech Republic; <sup>2</sup>Department of Biochemistry, Faculty of Science, Charles University, Prague 2, Czech Republic
- MP 434 **Optimized Clustering and Neighbor-Informed Re-identification of Spectra in a Spectral Archive by Complete Pair-wise Similarity Calculations and DBSCAN Clustering;** Ayman Hoque<sup>1</sup>; Henry Lam<sup>1</sup>; <sup>1</sup>Hong Kong University of Science and Technology, HONG KONG, Hong Kong
- MP 435 **DeepCCS: Context-aware prediction of peptide collisional cross section increases peptide recovery for out-of-distribution data-independent acquisition (DIA) datasets;** George Rosenberger<sup>1,2</sup>; Ignacio Jáuregui Novo<sup>2,3</sup>; Alexandros Pachos<sup>2</sup>; An-phi Nguyen<sup>2</sup>; Tejas Gandhi<sup>2</sup>; Dennis Trede<sup>4</sup>; Lukas Reiter<sup>2</sup>; <sup>1</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>2</sup>Biognosys AG, Schlieren, Switzerland; <sup>3</sup>Mestrelab Research S.L., Santiago de Compostela, Spain; <sup>4</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- MP 436 **Toward Massively Pooled Screens of Covalent Ligands Using a New Multi-Modification Comet Search;** Keon Hean Ooi<sup>1</sup>; Jimmy Eng<sup>2</sup>; Ramin Rad<sup>1</sup>; Ka Yang<sup>1</sup>; Brandon Gassaway<sup>3</sup>; Steven Shuken<sup>1</sup>; Julian Mintseris<sup>1</sup>; Qing Yu<sup>1</sup>; Joao A. Paulo<sup>1</sup>; Edward L. Huttlin<sup>1</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup>Harvard Medical School, Boston, MA; <sup>2</sup>Washington University in Saint Louis, St. Louis, MO; <sup>3</sup>Brigham Young University, Provo, UT
- MP 437 **DeIPI: Genuine library-free peptide identification in DIA data through deep feature learning;** Jungkap Park<sup>1</sup>; Dhonggeon Won<sup>1</sup>; Dmitry Avtonomov<sup>2</sup>; Sangtae Kim<sup>2</sup>; <sup>1</sup>Bertis Inc, Seoul, South Korea; <sup>2</sup>Bertis Bioscience, SAN DIEGO, CA
- MP 438 **Data-independent acquisition represents a promising alternative for FPOP samples analysis;** Marek Zakopcanik<sup>1,2</sup>; Dmitry S. Loginov<sup>1</sup>; Daniel Kavan<sup>1</sup>; Petr Novak<sup>1</sup>; <sup>1</sup>Institute of Microbiology of the Czech Academy of Sciences, 142 20, Prague, Czech Republic; <sup>2</sup>Department of Biochemistry, Charles University, Prague, Czech Republic
- MP 439 **Toward In-Depth MS1 Analysis of MS-Based Proteomics with PepPre2;** Ching Tarn<sup>1</sup>; Kai-Fei Wang<sup>1</sup>; Hao Chi<sup>1</sup>; <sup>1</sup>Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China
- MP 440 **PiQuant: software for rapid and accurate quantification of mass spectrometry-based proteomics data;** Pedro Moreno Cardoso<sup>1</sup>; David N. Perkins<sup>1</sup>; Nazrath Nawaz<sup>1</sup>; Weronika S. Borek<sup>1</sup>; Josie A. Christopher<sup>1</sup>; Amy E. Campbell<sup>1</sup>; Andrew Williamson<sup>1</sup>; Pedro R. Cutillas<sup>1,2</sup>; Arran D. Dokal<sup>1</sup>; <sup>1</sup>Kinomica Ltd, Macclesfield, Cheshire, United Kingdom; <sup>2</sup>Barts Cancer Institute, Queen Mary University of London, London, United Kingdom
- MP 441 **Sunshine and rainbows: constructive interference and the deconvolution of peptide MS1 spectra;** Florian Seefried<sup>1</sup>; Alexander Högge<sup>1</sup>; Patroklos Samaras<sup>1</sup>; Michael Graber<sup>1</sup>; Michelle T Berger<sup>1</sup>; Daniel P Zolg<sup>1</sup>; Mathias Wilhelm<sup>2</sup>; Martin Frejno<sup>1</sup>; <sup>1</sup>MSAID, Garching, Germany; <sup>2</sup>Technical University of Munich, Computational Mass Spectrometry, Freising, Germany
- MP 442 **MS1-based feature generation to improve identification rate in single cell proteomics datasets;** Sam Van Puyenbroeck<sup>1,2</sup>; Arthur Declercq<sup>1,2</sup>; Tine Claeys<sup>1,2</sup>; Ralf Gabriels<sup>1,2</sup>; Lennart Martens<sup>1,2</sup>; <sup>1</sup>VIB - UGent Center for Medical Biotechnology, Gent, Belgium; <sup>2</sup>Department of Biomolecular Medicine, Ghent University, Ghent, Belgium
- MP 443 **Peptide ancestral-informative markers for inferring the proportion of ancestry;** Yurou Huang<sup>1</sup>; Keyue Ding<sup>2</sup>; Songfeng Wu<sup>3</sup>; Yunping Zhu<sup>1</sup>; <sup>1</sup>State Key Laboratory of Medical Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences (Beijing), Beijing Institute of Lifeomics, Beijing, China; <sup>2</sup>Department of Cardiovascular Medicine, Mayo Clinic, Rochester, MN; <sup>3</sup>Beijing Qinglian Biotech Co., Ltd., Beijing, China
- MP 444 **Big Data, Small Organisms: A holistic view on the community-wide assembled E. coli Proteome;** Caroline Jachmann<sup>1,2</sup>; Aurélie Hirschler<sup>3</sup>; Florence Arsène-Ploetze<sup>4</sup>; Christine Carapito<sup>3</sup>; Luis Mendoza<sup>5</sup>; Eric W Deutsch<sup>5</sup>; Zhi Sun<sup>5</sup>; Ralf Gabriels<sup>1,2</sup>; Robbin Bouwmeester<sup>1,2</sup>; Kay Nieselt<sup>6</sup>; Tim Van Den Bossche<sup>1,2</sup>; Lennart Martens<sup>1,2</sup>; <sup>1</sup>VIB-UGent Center for Medical Biotechnology, VIB, Ghent, Belgium; <sup>2</sup>Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; <sup>3</sup>BioOrganic Mass Spectrometry Laboratory (LSMBO), IPHC UMR 7178, University of Strasbourg, CNRS, ProFI, Strasbourg, France; <sup>4</sup>Institut de biologie moléculaire des plantes, CNRS, Université de Strasbourg, Strasbourg, France; <sup>5</sup>Institute for Systems Biology, Seattle, Washington; <sup>6</sup>Institute for Bioinformatics and Medical Informatics, University of Tübingen, Sand 14, 72076, Tübingen, Germany
- MP 445 **Pioneer: Fast and Open-Source Algorithms for Analyzing Data-Independent Acquisition Proteomics Experiments;** Nathan T Wamsley<sup>1</sup>; Michael B Major<sup>1</sup>; Dennis Goldfarb<sup>1</sup>; <sup>1</sup>Washington University in Saint Louis, St. Louis, MO
- MP 446 **Oktoberfest: search engine agnostic rescoring pipeline leveraging online peptide property prediction from various models;** Mario Picciani<sup>1,2</sup>; Wassim Gabriel<sup>1</sup>; Ludwig Lautenbacher<sup>1</sup>; Armin Soleymaniyani<sup>1,2</sup>; Xiao Zixuan<sup>1</sup>; Eva Ayla Schroeder<sup>1</sup>; Matthew The<sup>3</sup>; Mostafa Kalhor<sup>1</sup>; Charlotte Adams<sup>4</sup>; Wout Bittremieux<sup>4</sup>; Kurt Boonen<sup>5</sup>; Mathias Wilhelm<sup>1,2</sup>; <sup>1</sup>Computational Mass Spectrometry, TUM, Freising, Germany; <sup>2</sup>Elite Network Bavaria, TUM, Freising, Germany; <sup>3</sup>Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; <sup>4</sup>Department of Computer Science, University of Antwerp, Antwerp, Belgium; <sup>5</sup>Department of Biomedical Sciences, University of Antwerp, Antwerp, Belgium
- MP 447 **tims2Rescore: A DDA-PASEF optimized data-driven identification rescoring pipeline;** Arthur Declercq<sup>1,2</sup>; Robbe Devreese<sup>1,3</sup>; Jonas Scheid<sup>4,5,6</sup>; Caroline Jachmann<sup>1,3</sup>; David Gomez-Zepeda<sup>7,8,9</sup>; Jeewan Babu RIJAL<sup>10</sup>; Aurélie Hirschler<sup>10</sup>; Jonathan R Krieger<sup>11</sup>; Tharan Srikumar<sup>11</sup>; George Rosenberger<sup>12</sup>; Dennis Trede<sup>13</sup>; Christine Carapito<sup>10</sup>; Stefan Tenzer<sup>7,8,14,15</sup>; Juliane Walz<sup>4,5,16</sup>; Sven Degroeve<sup>1,3</sup>; Robbin Bouwmeester<sup>1,3</sup>; Lennart Martens<sup>1,3</sup>; Ralf Gabriels<sup>1,3</sup>; <sup>1</sup>VIB / UGent - Center for Medical Biotechnology (CMB), Ghent, Belgium; <sup>2</sup>Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; <sup>3</sup>Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; <sup>4</sup>Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tübingen, Tübingen, Germany; <sup>5</sup>Cluster of Excellence iFIT (ECX2180) "Image-Guided and Functionally Instructed Tumor Therapies"; University of Tuebingen, Tuebingen, Germany;

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- MP 448 **Spectrum-centric and acquisition method-agnostic deconvolution of tandem mass spectra improves the identification and site localization of acetylated and ubiquitinated peptides**; Daniel P Zolg<sup>1</sup>; Tobias Schmidt<sup>1</sup>; Siegfried Gessulat<sup>2</sup>; Florian Seefried<sup>1</sup>; Michael Graber<sup>1</sup>; Samia Ben Fredj<sup>1</sup>; Patroklos Samaras<sup>1</sup>; Markus Schneider<sup>1</sup>; Layla Eljagh<sup>1</sup>; Vishal Sukumar<sup>1</sup>; Michelle T Berger<sup>1</sup>; Alexander Hogrebe<sup>2</sup>; Igor Bronshtein<sup>2</sup>; Pedro Navarro<sup>3</sup>; Kai Fritze<sup>3</sup>; Yovany Cordero Hernandez<sup>3</sup>; Frank Berg<sup>3</sup>; Carmen Paschke<sup>3</sup>; David M Horn<sup>4</sup>; Philip L Loziuk<sup>4</sup>; Bernard Delanghe<sup>3</sup>; Christoph Henrich<sup>3</sup>; Martin Heinrich Frejno<sup>1</sup>; <sup>1</sup>MSAID, Garching, Germany; <sup>2</sup>MSAID, Berlin, Germany; <sup>3</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; <sup>4</sup>Thermo Fisher Scientific, San Jose, CA
- MP 449 **FragPipe Advancements for Optimized DDA, DDA+, and DIA Mass Spectrometry Data Analysis**; Fengchao Yu<sup>1</sup>; Yamei Deng<sup>1</sup>; Daniel A. Polasky<sup>1</sup>; Kevin L. Yang<sup>1</sup>; Kai Li<sup>1</sup>; Guo Ci Teo<sup>1</sup>; Alexey I. Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, Michigan
- MP 450 **De novo sequencing of multiple peptides in chimeric mass spectra**; Yanik Bruns<sup>1</sup>; Mathias Wilhelm<sup>2, 3</sup>; Julien Gagneur<sup>1, 3, 4, 5</sup>; <sup>1</sup>Computational Molecular Medicine, School of Computation, Information and Technology, Technical University of Munich, Munich, Germany; <sup>2</sup>Computational Mass Spectrometry, TU Munich, TUM School of Life Sciences, Freising, Germany; <sup>3</sup>Munich Data Science Institute, Technical University of Munich, Garching bei Muenchen, Germany; <sup>4</sup>Institute of Human Genetics, School of Medicine, Technical University of Munich, Munich, Germany; <sup>5</sup>Computational Health Center, Helmholtz Center Munich, Neuherberg, Germany
- MP 451 **Confident identification of proteome-wide low-level mutations using PEAKS 11.5**; Kyle Hoffman<sup>1</sup>; Julie Genereaux<sup>2</sup>; Lei Xin<sup>1</sup>; Zia Rahman<sup>1</sup>; Christopher J Brandt<sup>2</sup>; Patrick O'Donoghue<sup>2</sup>; Baozhen Shan<sup>1</sup>; <sup>1</sup>Bioinformatics Solutions Inc., Waterloo, ON; <sup>2</sup>Western University, London, Ontario
- MP 452 **The Synergistic Effect of combining ProSIT rescoring with SIMSI-Transfer for Clinical Cancer Cohorts**; Firas Hamood<sup>1</sup>; Pia Pfeiffer<sup>1</sup>; Wassim Gabriel<sup>1</sup>; Mathias Wilhelm<sup>1</sup>; Bernhard Kuster<sup>1</sup>; Matthew The<sup>1</sup>; <sup>1</sup>Technical University of Munich (TUM), Freising, Germany
- MP 453 **Improving single-cell data interpretation by joint modeling of peptide fragmentation spectra**; Kevin McDonnell<sup>1</sup>; Harrison Specht<sup>1</sup>; Nikolai Slavov<sup>1, 2</sup>; <sup>1</sup>Parallel Squared Technology Institute, Watertown, MA; <sup>2</sup>Northeastern University, Boston, MA
- MP 454 **Conceptual Framework for SCP Chimeric Spectra Annotation**; Alyssa A Nitz<sup>1</sup>; Samuel H Payne<sup>1</sup>; <sup>1</sup>Brigham Young University, Provo, UT
- MP 455 **Fragment ion indexing accelerates Comet database search and expands real-time search capabilities**; Erik J Bergstrom<sup>1</sup>; Jimmy Eng<sup>1</sup>; Chris McGann<sup>1</sup>; Fengchao Yu<sup>2</sup>; Qing Yu<sup>3</sup>; Alexey I Nesvizhskii<sup>2</sup>; Devin K Schweppe<sup>1</sup>; <sup>1</sup>University of Washington - Genome Sciences, Seattle, WA; <sup>2</sup>University of Michigan, Ann Arbor, MI; <sup>3</sup>Harvard Medical School, Boston, MA
- MP 456 **Integrative bioinformatic analysis of human lysine ubiquitylation provides insight into strategies for comprehensive site-localized ubiquitylomics**; Regina M. Edgington<sup>1</sup>; Damien B Wilburn<sup>2</sup>; <sup>1</sup>The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; <sup>2</sup>The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio
- ION MOBILITY: APPLICATIONS I**  
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- MP 457 **Flow injection analysis of isomers of new psychoactive substances using cyclic ion mobility mass spectrometry**; Marianna Nytká<sup>1</sup>; František Tureček<sup>2</sup>; Karel Lemr<sup>1</sup>; <sup>1</sup>Department of Analytical Chemistry, Faculty of Science, Palacký University, Tr. 17. listopadu 12, 779 00, Olomouc, Czech Republic; <sup>2</sup>Department of Chemistry, University of Washington, Seattle, WA
- MP 458 **Implementation of native RapidFire ion mobility mass spectrometry (nRF-IM-MS) for assessment of the higher order structure (HOS) stability of biotherapeutics**; Max Shih<sup>1</sup>; Patrick J Faustino<sup>1</sup>; Xiaoming Xu<sup>1</sup>; Jinhui Zhang<sup>1</sup>; <sup>1</sup>Food and Drug Administration, Silver Spring, MD
- MP 459 **A Collision-Induced Dissociation-Trap Ion Mobility (CID-TIMS) Workflow for Site-Specific Identification of Isomerized Residues in Neuropeptides**; Samuel Okyem<sup>1, 2</sup>; Jonathan V Sweedler<sup>1, 2</sup>; <sup>1</sup>University of Illinois-Urbana Champaign, Urbana, IL; <sup>2</sup>Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Champaign, IL
- MP 460 **Online radioligand therapy reaction monitoring optimization and chelation efficiency by cyclic ion mobility spectrometry-mass spectrometry**; Brooke Brown<sup>1</sup>; Samuel Annan<sup>1</sup>; Rohit Duvadie<sup>1</sup>; Richard Robinson<sup>1</sup>; <sup>1</sup>Novartis Biomedical Research, Cambridge, MA
- MP 461 **Exploring Ion Mobility Data File Conversions to Leverage Existing Tools and Enable New Workflows**; Sarah M. Stow<sup>1</sup>; Hannah Florance<sup>1</sup>; David A. Weil<sup>1</sup>; Bryson Gibbons<sup>2</sup>; Aivett Bilbao<sup>2</sup>; Richard Knochenmuss<sup>3</sup>; Ruwan T. Kurulugama<sup>1</sup>; John C. Fjeldsted<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>3</sup>RKResearch, Seftigen, Switzerland
- MP 462 **Enhancing Host Cell Protein (HCP) Analysis using SLIM-based Orbitrap Platform**; Liulin Deng<sup>1</sup>; Alan McKenzie-Coe<sup>1</sup>; Greg Kilby<sup>1</sup>; Kyle L. Fort<sup>2</sup>; Brian Adamson<sup>3</sup>; Oliver M Bernhardt<sup>4</sup>; Roland Bruderer<sup>4</sup>; Tejas Gandhi<sup>4</sup>; Lukas Reiter<sup>4</sup>; Eloy R. Wouters<sup>3</sup>; Jean-Jacques Dunyach<sup>3</sup>; Daniel DeBord<sup>1</sup>; Alexander A. Makarov<sup>2</sup>; <sup>1</sup>MOBILion Systems, Chadds Ford, PA; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA; <sup>4</sup>Biognosys AG, Schlieren, Switzerland
- MP 463 **Nucleotide derivative isomers analysis using ion mobility spectrometry and theoretical calculations**; Chuan-Fan Ding<sup>1</sup>; Fangling Wu<sup>1</sup>; <sup>1</sup>Ningbo University, Ningbo, China
- MP 464 **An Ion Mobility Collision Cross Section Database in Support of the Periodic Table of Food Initiative**; Jody C May<sup>1</sup>; Katrina L Leaptrot<sup>1</sup>; Chi-Ming Chien<sup>2</sup>; Tracy Shafizadeh<sup>2</sup>; Steve Watkins<sup>2</sup>; Stacy D Sherrod<sup>1</sup>; John A McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Verso Biosciences, Davis, CA
- MP 465 **Assessing selectivity of deubiquitinating enzymes via ion mobility-based analysis of polyubiquitin isomers**; Elizaveta Shestoperova<sup>1</sup>; Eric R Strieter<sup>1</sup>; <sup>1</sup>University of Massachusetts Amherst, Amherst, MA
- MP 466 **The Utility of Cyclic Ion Mobility to Improve Selectivity and Analysis Efficiency of Environmental PFAS Contamination and Exposure**; Michael McCullagh<sup>1</sup>; Logy Kass<sup>2</sup>; Georgios Theodoridis<sup>3</sup>; Artemis Lioupi<sup>3</sup>; Robert

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- Plumb<sup>2</sup>; Sarah Dowd<sup>4</sup>; Stuart Adams<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Waters Corporation, Milford, MA; <sup>3</sup>Laboratory of Analytical Chemistry, School of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece; <sup>4</sup>Waters, Milford, MA
- MP 467 **Characterization using ion mobility MS and energy minimization modeling of conformational distinctions between mono- and diphosphorylated PIPs**; Hernando Olivos<sup>1</sup>; Prithviraj Nandigrama<sup>2</sup>; Steven Lai<sup>1</sup>; Christopher Jurtschenko<sup>1</sup>; Yunping Qiu<sup>2</sup>; Andras Fiser<sup>2</sup>; Irwin J. Kurland<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Albert Einstein College of Medicine, Bronx, NY
- MP 468 **In-depth investigation of PFAS occurrence in environmental samples combining LC-VIP HESI-TIMS-QTOF MS with PASEF and untargeted data processing**; Georgios Gkotsis<sup>1</sup>; Dimitrios E. Damalas<sup>1</sup>; Bob Galvin<sup>2</sup>; Carsten Baessmann<sup>3</sup>; Nikolaos S. Thomaidis<sup>1</sup>; <sup>1</sup>National and Kapodistrian University of Athens, Department of Chemistry, Laboratory of Analytical Chemistry, Athens, Greece; <sup>2</sup>Bruker Daltonics, Coventry, United Kingdom; <sup>3</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- MP 469 **Structural Characterization of Endogenous Endocrine Hormone Isomers using High-Resolution SLIM Ion Mobility**; Makenna K Hoover<sup>1</sup>; Christopher D. Chouinard<sup>1</sup>; <sup>1</sup>Clemson University, Clemson, SC
- MP 470 **Protein-Ligand Binding by Native Flow Injection Analysis and Native SEC Electrospray Ionization with High-Resolution Ion Mobility Mass Spectrometry (HRIM-MS)**; Greg W Kilby; MOBILion, Chadds Ford, PA
- MP 471 **Characterization of Microcystin Compounds Using High Resolution Ion Mobility Mass Spectrometry**; Esabella R Powers<sup>1</sup>; Jae Hwan Lee<sup>1,2</sup>; Michael W Christopher<sup>1</sup>; Krista McCoy<sup>3</sup>; Daniel DeBord<sup>4</sup>; Sarah M. Stow<sup>5</sup>; Ruwan T Kurulugama<sup>5</sup>; Boone M. Prentice<sup>1</sup>; Richard A Yost<sup>1</sup>; Timothy J. Garrett<sup>1,6</sup>; <sup>1</sup>Department of Chemistry, University of Florida, Gainesville, FL; <sup>2</sup>Air Force Institute of Technology, United States Air Force, Wright-Patterson AFB, OH; <sup>3</sup>Harbor Branch Oceanographic Institute, Florida Atlantic University, Fort Pierce, FL; <sup>4</sup>MOBILion Systems, Inc., Chadds Ford, PA; <sup>5</sup>Agilent Technologies, Santa Clara, CA; <sup>6</sup>Department of Pathology, Immunology and Laboratory Medicine and Southeast Center for Integrated Metabolomics, University of Florida, Gainesville, FL
- MP 472 **Collision Cross Section Prediction using Graph Neural Networks for improved compound identification**; Shaurya Chanana<sup>1</sup>; Chloe Engler Hart<sup>1</sup>; António José Preto<sup>1</sup>; Daniel Domingo-Fernandez<sup>1</sup>; Tobias Kind<sup>1</sup>; David Healey<sup>1</sup>; <sup>1</sup>Enveda Biosciences, Boulder, CO
- MP 473 **Enabling Protein and Oligonucleotide Ion Mobility Data Analysis in BioConfirm with PNNL Preprocessor Data Conversions**; Gordon W. Slys<sup>1</sup>; Sarah M. Stow<sup>2</sup>; Jack P. Ryan<sup>3</sup>; Erin S. Baker<sup>3</sup>; Rebecca Glaskin<sup>2</sup>; Michael D. Knierman<sup>2</sup>; Aivett Bilbao<sup>4</sup>; Bryson Gibbons<sup>4</sup>; Christian Klein<sup>2</sup>; Ruwan T. Kurulugama<sup>2</sup>; Crystal Cody<sup>2</sup>; John C. Feldsted<sup>2</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>University North Carolina at Chapel Hill, Chapel Hill, NC; <sup>4</sup>Pacific Northwest National Laboratory, Richland, WA
- MP 474 **Analysis of Gas Phase Protein Complex Unfolding in Positive and Negative nESI**; Martha Ortega Zepeda<sup>1,2</sup>; Yu-Fu Lin<sup>1,2</sup>; Dalton T Snyder<sup>2</sup>; Vicki H Wysocki<sup>1,2</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; <sup>2</sup>Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH
- MP 475 **Separation of Isobaric Amino acids and Small Molecule Metabolites Using Multipass Ion Mobility Analysis**; Hernando Olivos<sup>1</sup>; Jorge Smith<sup>1</sup>; Eve L Berger<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>National Aeronautics and Space Administration, Houston, TX
- MP 476 **Ride the Wave: Challenging Enantiomeric separation Using SLIM-Ion Mobility Mass Spectrometry**; Meenakshi Goel<sup>1</sup>; Sayyeda Zeenat A Razvi<sup>1</sup>; Jose G Napolitano<sup>2</sup>; Sreya Sarkar<sup>2</sup>; Christopher M Crittenden<sup>2</sup>; <sup>1</sup>Genentech Inc., South San Francisco, CA; <sup>2</sup>Genentech Inc, South San Francisco, CA

### LIPIDS: ID AND STRUCTURAL ANALYSIS I 477-496

- MP 477 **Aza-Prilezhaev Aziridination-Enabled Multidimensional Analysis of Isomeric Lipids via High-Resolution U-Shaped Mobility Analyzer-Mass Spectrometry**; Yuling Li<sup>1</sup>; Yiming Wang<sup>1</sup>; Kang Guo<sup>1</sup>; Kuofeng Tseng<sup>1</sup>; Xiaoqiang Zhang<sup>1</sup>; Wenjian Sun<sup>1</sup>; <sup>1</sup>Shimadzu Research Laboratory (Shanghai) Co. Ltd., Shanghai, China
- MP 478 **Isomer-resolving CE-MS enables comprehensive analysis of lipidome in single cell spheroids**; Wenpeng Zhang<sup>1</sup>; Junhan Wu<sup>2</sup>; Yikun Liu<sup>1</sup>; Zheng Ouyang<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>PURSPEC Technology (China) Ltd., Suzhou, China
- MP 479 **Identification of Double Bond Positions in Ceramides from the Stratum Corneum Using OAD-TOF System**; Yohei Arai<sup>1</sup>; Mami Okamoto<sup>1</sup>; Hidenori Takahashi<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Nakagyo-ku, Japan
- MP 480 **Structural Elucidation of Copper-complexed Phosphatidylcholines via Tandem Mass Spectrometry**; Zunaira Naeem<sup>1</sup>; Tingting Yan<sup>2</sup>; Julia R. Bonney<sup>2</sup>; Boone M. Prentice<sup>2</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>University of Florida, GAINESVILLE, FL
- MP 481 **Characterization of Lipid Isomers Observed During Lipidomic LX-MS via Ozone-Induced Dissociation Mass Spectrometry (OzID-MS)**; Kimber N. Focke<sup>1</sup>; James D. Sanders<sup>1</sup>; Michael T. Marty<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ
- MP 482 **Data independent acquisition coupled with electron activated dissociation for hydroxy position resolved profiling of FAHFA**; Yuto Kurizaki<sup>1</sup>; Yuki Matsuzawa<sup>1</sup>; Kanako Tokiyoshi<sup>1</sup>; Hiroaki Takeda<sup>1</sup>; Mayu Hasegawa<sup>2</sup>; Junki Miyamoto<sup>2</sup>; Mikiko Takahashi<sup>3</sup>; Hiroshi Tsugawa<sup>1,3</sup>; <sup>1</sup>Tokyo University of Agriculture and Technology, Koganei-shi, Japan; <sup>2</sup>Tokyo University of Agriculture and Technology, Fuchu, Japan; <sup>3</sup>RIKEN Center for Sustainable Resource Science, Yokohama, Japan
- MP 483 **An Integrated MS-Based Platform for Structure-Based Identification and Quantification of Glycosphingolipids**; Ji Eun Park<sup>1,2</sup>; Myung Jin Oh<sup>1,2</sup>; Hyun Joo An<sup>1,2</sup>; <sup>1</sup>Chungnam National University, Daejeon, South Korea; <sup>2</sup>Asia-Pacific Glycomics Reference Site, Daejeon, South Korea
- MP 484 **Identifying Oxidized Glycolipids in Microalgae: Bridging LC-MS Lipidomics with Biological Roles**; Rosario Domingues<sup>1</sup>; Tiago Conde<sup>1</sup>; Diana Lopes<sup>1</sup>; Tânia Melo<sup>1</sup>; Pedro Domingues<sup>1</sup>; <sup>1</sup>University of Aveiro, Aveiro, Portugal
- MP 485 **Lipid Characterization Using MS Imaging and LCMS in Liver of a Metabolic Dysfunction-Associated Steatohepatitis (MASH) Mouse Model**; Doug Carlton<sup>1</sup>; Jeff Dahl<sup>1</sup>; Ruth Gordillo<sup>2</sup>; Toshiya Matsubara<sup>1</sup>; Christine Kusminski<sup>2</sup>; Kyounghee Min<sup>2</sup>; Philipp E Scherer<sup>2</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>2</sup>University of Texas Southwestern Medical Center, Dallas, TX
- MP 486 **Metabolic Degradation and Global Lipidome Incorporation of Polyfluorinated Model Decanes in Pseudomonas sp. Strain 273**; Alexander S Walls<sup>1,2</sup>; Gao Chen<sup>3,4</sup>; Diana Ramirez<sup>3,4</sup>; Frank E Loeffler<sup>3,4,5,6</sup>; Shawn R. Campagna<sup>1,2</sup>; <sup>1</sup>University of Tennessee Knoxville Chemistry Dept., Knoxville, TN; <sup>2</sup>Biological Small Molecule Mass Spectrometry Core, Knoxville, TN; <sup>3</sup>University of Tennessee, Knoxville, TN; <sup>4</sup>Department of Microbiology, Knoxville, TN; <sup>5</sup>Department of Civil and Environmental Engineering, Knoxville, TN; <sup>6</sup>Department of Biosystems Engineering and Soil Science, Knoxville, TN
- MP 487 **Efficient Multimodal MS Data Analysis with MZmine: Unraveling Lipid A Composition in Pathological E. coli**; Ansgar Korf<sup>1</sup>; Edward Rudt<sup>2</sup>; Steffen Heuckeroth<sup>1</sup>; Robin Schmid<sup>3</sup>; Tomáš Pluskal<sup>3</sup>; Heiko Hayen<sup>2</sup>; <sup>1</sup>mzio GmbH, Bremen, Germany; <sup>2</sup>University of Münster, Institute of

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- Inorganic and Analytical Chemistry, Münster, Germany;*  
<sup>3</sup>*Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic*
- MP 488 **Automated and detailed structural elucidation of lipids in biological matrix;** Pradeep Narayanaswamy<sup>1</sup>; Eva Duchoslav<sup>2</sup>; Pavel Ryumin<sup>2</sup>; <sup>1</sup>SCIEX, Singapore, Singapore; <sup>2</sup>SCIEX, Concord, ON
- MP 489 **Measuring the entropies and enthalpies of activation of sn-1/sn-2 acyl chain loss in six glycerophospholipid classes using dipolar DC kinetics;** Samantha A Mehnert<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- MP 490 **Identification of positional isomers of linoleic acid containing phospholipids involved in pancreatic ductal adenocarcinoma;** Emily G Armitage<sup>1</sup>; Alan Barnes<sup>1</sup>; Elon Correa<sup>2</sup>; S en Takeda<sup>3</sup>; Wen Chung<sup>4</sup>; Neil J Loftus<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Manchester, United Kingdom; <sup>2</sup>Liverpool John Moores University, Liverpool, United Kingdom; <sup>3</sup>Department of Anatomy, Teikyo University School of Medicine, Tokyo, Japan; <sup>4</sup>Leicester HPB Unit, Glenfield Hospital, Leicester, United Kingdom
- MP 491 **Post Column Epoxidation for Differentiating Polar and Non-polar Lipids Isomers via Liquid Chromatography Co-axial Contained-ESI Mass Spectrometry;** Niraj K. Panday<sup>1</sup>; Alexander J. Grooms<sup>1</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH
- MP 492 **A decision tree approach for triacylglycerol annotation of data-independent acquisition based lipidomics data;** Victor CL Lee<sup>1</sup>; Khanh CK Nguyen<sup>1</sup>; Thomas J Velenosi<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, BC
- MP 493 **Large-scale lipidome analysis at the isomer-resolving level based on Omega Analyzer;** Junhan Wu<sup>1</sup>; Wenhui Pang<sup>1</sup>; Hongzheng Zhou<sup>1</sup>; Jiexun Bu<sup>2</sup>; Wenpeng Zhang<sup>3</sup>; Zheng Ouyang<sup>3</sup>; <sup>1</sup>PURSPEC Technology(China) Ltd., Suzhou, China; <sup>2</sup>PURSPEC Technology (Beijing) Ltd., Beijing, China; <sup>3</sup>Tsinghua University, Beijing, China
- MP 494 **Evaluation of the synthesis of the branched chain ionizable lipid C12-200 using LC-MS/MS with low-energy electron impact fragmentation;** Daniel Zimmer<sup>1</sup>; Matthew D. Stone<sup>2</sup>; Robert Proos<sup>2</sup>; Santosh Kapil Kumar Gorti<sup>2</sup>; Christina Bailey-Hytholt<sup>1</sup>; <sup>1</sup>Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MASSACHUSETTS; <sup>2</sup>SCIEX, USA, Framingham, MASSACHUSETTS
- MP 495 **Embrace both worlds: manipulating ion-types via gas-phase ion chemistry for structural elucidation of sugar-lipid conjugates;** Hsi-Chun Chao<sup>1, 2</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>University of Illinois Urbana-Champaign, Champaign, IL
- MP 496 **Utilizing Normal Phase Amino Columns in Chromatography for Enhanced Discrimination of Charged, Chargedecayed, and Uncharged Modifications in Glycolipid and Glycan;** Akio Hayashi<sup>1</sup>; Takashi Matsuzaka<sup>2</sup>; Hitoshi Shimano<sup>3</sup>; <sup>1</sup>Osaka University, Center for Infectious Disease Education and Research, Suita, Japan; <sup>2</sup>Department of Endocrinology and Metabolism, Faculty of Medicine, University of Tsukuba, Tsukuba, Japan; <sup>3</sup>Department of Endocrinology and Metabolism, Faculty of Medicine, University of Tsukuba, Tsukuba, Japan
- LIPIDS: PROFILE ANALYSIS**  
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- MP 497 **Tailored Cardiolipin Analysis in Complex Biological Matrices by two-dimensional HPLC coupled to high-resolution mass spectrometry;** Vera Schwantes<sup>1</sup>; Ann-Kathrin Weishaupt<sup>2</sup>; Julia Bornhorst<sup>2</sup>; Heiko Hayen<sup>1</sup>; <sup>1</sup>University of M nster, Department of Inorganic and Analytical Chemistry, M nster, Germany; <sup>2</sup>University of Wuppertal, Faculty of Mathematics and Natural Sciences, Wuppertal, Germany
- MP 498 **Age-dependent changes in mouse brain and liver lipidomes;** Punyatoya Panda<sup>1</sup>; Christina R. Ferreira<sup>2</sup>; Allison Schaser<sup>3</sup>; Uma K. Aryal<sup>1, 2</sup>; <sup>1</sup>Department of Comparative Pathobiology, Purdue University, West Lafayette, Indiana; <sup>2</sup>Bindley Bioscience Center, Purdue University, West Lafayette, Indiana; <sup>3</sup>Department of Speech, Language, and Hearing Sciences, Purdue University, West Lafayette, Indiana
- MP 499 **Bridging Gaps in Honey Bee Pheromone Analysis Using State-of-the-Art Lipidomics Analysis;** Armando Alcazar Magana<sup>1, 2</sup>; Alison McAfee<sup>1, 3</sup>; Shelley E. Hoover<sup>4</sup>; Leonard J Foster<sup>1, 2</sup>; <sup>1</sup>Michael Smith Laboratories, Department of Biochemistry and Molecular Biology, University of British Columbia, Vancouver, British Columbia; <sup>2</sup>Life Sciences Institute, Department of Biochemistry and Molecular Biology, University of British Columbia, Vancouver, British Columbia; <sup>3</sup>Department of Applied Ecology, North Carolina State University, Raleigh, North Carolina; <sup>4</sup>Department of Biological Sciences, University of Lethbridge, Lethbridge, Alberta
- MP 500 **Untargeted Lipidomics of Murine Plasma Extracellular Vesicles;** Paul D Kennedy<sup>1</sup>; Brooke Saepoo<sup>1</sup>; Dilrukshika S.W. Palagama<sup>2</sup>; Miguel A. Gijon<sup>1</sup>; Elizabeth A. Hurst<sup>1</sup>; David LaGory<sup>1</sup>; <sup>1</sup>Cayman Chemical Company, Ann Arbor, MI; <sup>2</sup>Cayman Chemical Company, Cayman Chemical Company, MI
- MP 501 **Investigating the Effects of Alteration in Lipid Profile on Biological Pathways in Diabetic Patients Treated with Different Drugs;** Waziha Tasnim Purba<sup>1</sup>; Shams Tarek Osman<sup>2</sup>; Oluwatosin Daramola<sup>1</sup>; Judith Nwaiwu<sup>1</sup>; Md Mostofa Al Amin Bhuiyan<sup>1</sup>; Mojibola Fowowe<sup>1</sup>; Junyao Wang<sup>1</sup>; Ahmed Elyazbi<sup>3</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; <sup>2</sup>Department of Clinical Pharmacy and Pharmacy Practice, Faculty of Pharmacy, Alexandria University, Alexandria, Egypt; <sup>3</sup>Department of Pharmacology and Therapeutics, Faculty of Pharmacy, Alamein International University, Alamein, Egypt
- MP 502 **High Throughput Profiling Method for Comprehensive Lipidomics Analysis of Samples of Limited Amounts;** Ya-Chun Chan<sup>1</sup>; Xiaohang Wang<sup>1</sup>; Shuang Zhao<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta
- MP 503 **Effects of a High-Fat Diet on Triacylglycerols in Adipose Tissue in a GHSR KO Rat Model;** Lindsay A Kryszak<sup>1</sup>; Shelley N Jackson<sup>1</sup>; Andras H Leko<sup>1</sup>; Adriana Gregory-Flores<sup>1</sup>; Renata C N Marchette<sup>1</sup>; Janaina C M Vendruscolo<sup>1</sup>; Leandro F Vendruscolo<sup>1</sup>; Lorenzo Leggio<sup>1</sup>; <sup>1</sup>National Institute on Drug Abuse, Baltimore, MD
- MP 504 **LC-MS Characterization of Lipid Nanoparticle Components and Relevant Major Cholesterol Oxidation Products;** Kevin Ray<sup>1</sup>; Katherine Sanders<sup>1</sup>; <sup>1</sup>MilliporeSigma, St. Louis, MO
- MP 505 **Analyzing sex-dependent effects of bisphenol A on hepatic lipid metabolism in zebrafish using UPLC-Q-TOF/MS;** Won Noh<sup>1</sup>; <sup>1</sup>Korea institute of Toxicology, Jinju, South Korea
- MP 506 **Time-dependent Investigation of Formation of Serum Biomolecular Coronas around Nanoparticles for Nanomedicine;** Gwi Ju Jang<sup>1</sup>; Min A Kim<sup>1</sup>; Heeju Joung<sup>1</sup>; Sang Yun Han<sup>1</sup>; <sup>1</sup>Department of chemistry, Gachon University, Seongnam-si, South Korea
- MP 507 **Vendor-dependent mobile phase contaminants affect neutral lipid detection in lipidomics analyses;** Joshua A Roberts<sup>1</sup>; Angela S Radnoff<sup>1</sup>; Aleksandra Bushueva<sup>1</sup>; Jocelyn A Menard<sup>1</sup>; Karl V Wasslen<sup>1</sup>; Meaghan Harley<sup>1</sup>; Jeffrey M Manthorpe<sup>1</sup>; Jeffrey C Smith<sup>1</sup>; <sup>1</sup>Department of Chemistry, Carleton University, Ottawa, ON
- MP 508 **MRM based free fatty acids profiling in human plasma using LC-MS/MS;** Yuki Suzuki<sup>1</sup>; Naoko Nagano<sup>2</sup>; Takahiro Goda<sup>1</sup>; Masaki Yamada<sup>3</sup>; <sup>1</sup>SHIMADZU Corporation, Kawasaki, Japan; <sup>2</sup>Shimadzu General Services, Inc., Kyoto, Japan; <sup>3</sup>Shimadzu Corporation, Kyoto, Japan
- MP 509 **Distinct Polar Lipid Profiles in Fatty Acid Oxidation Disorders Identified by Dried Blood Spot Lipidomics;**

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- Inês M. S. Guerra<sup>1,2</sup>; Hugo Rocha<sup>3,4</sup>; Tânia Melo<sup>1,2</sup>; Ana S. P. Moreira<sup>2</sup>; M. Rosário Domingues<sup>1,2</sup>; Pedro Domingues<sup>1</sup>; <sup>1</sup>Mass Spectrometry Center, LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, Aveiro, Portugal; <sup>2</sup>CESAM-Centre for Environmental and Marine Studies-, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, , Portugal, Aveiro, Portugal; <sup>3</sup>Newborn Screening, Metabolism and Genetics Unit, Human Genetics Department, National Institute of Health Doutor Ricardo Jorge, Porto, Portugal; <sup>4</sup>Department of Pathological, Cytological and Thanatological Anatomy, School of Health, Polytechnic Institute of Porto, Porto, Portugal
- MP 510 **LIPIDOMICS OF SICKLE CELL DISEASE AND LIPID PROFILING OF ERYTHROCYTES-NOVEL FINDING;** Prasanth Kumar Punathil Kannan<sup>1</sup>; Sugasini Dhavamani<sup>2</sup>; Anuj Tiwari<sup>3</sup>; Jagadeesh Ramasamy<sup>1</sup>; <sup>1</sup>Department of Pediatrics, University of Illinois at Chicago, Chicago, IL; <sup>2</sup>University of Illinois, Chicago, IL; <sup>3</sup>Discovery Partners Institute, Chicago, IL
- MP 511 **Non-targeted lipidomics of human plasma for discovering biomarkers in thrombogenesis;** Chau Tran<sup>1</sup>; Daniil G. Ivanov<sup>1</sup>; Sina Farzaneh<sup>1</sup>; Juan M. Jiménez<sup>2</sup>; Evgenii Serebriakov<sup>1</sup>; Igor A. Kaltashov<sup>1</sup>; <sup>1</sup>University of Massachusetts Amherst, Amherst, MA
- MP 512 **Differences in the diet of calves detected in beef samples using surface extraction and multiple reaction monitoring profiling of lipids;** Juliana A Torrecilhas<sup>1</sup>; Gislaine Dos Santos<sup>2,3</sup>; Tiago J P Sobreira<sup>3</sup>; Sage Y Min<sup>4</sup>; Bruce R Cooper<sup>3</sup>; Rogério A Curi<sup>5</sup>; Luis A Chardulo<sup>1,5</sup>; Luciana M Sousa<sup>1,5</sup>; Flavio D Resende<sup>5</sup>; Gustavo R Siqueira<sup>5</sup>; Guilherme L Pereira<sup>1,5</sup>; Christina R Ferreira<sup>3</sup>; <sup>1</sup>College of Veterinary and Animal Science, University of São Paulo State Júlio de Mesquita Filho, Botucatu, Brazil; <sup>2</sup>Department of Veterinary Medicine, College of Animal Sciences and Food Engineering, University of São Paulo, Pirassununga, Brazil; <sup>3</sup>Bindley Bioscience Center, Purdue University, West Lafayette, Indiana; <sup>4</sup>Department of Biomedical Engineering, Purdue University, West Lafayette, Indiana; <sup>5</sup>College of Agronomics and Veterinary Sciences, University of São Paulo State Júlio de Mesquita Filho, Jaboticabal, Brazil
- MP 513 **Untargeted Lipidomics Pipeline for 3rd Generation Lentiviral Vectors and Packaging Cells;** Jocelyn A Menard<sup>1</sup>; Joshua A Roberts<sup>1</sup>; Elena Godbout<sup>2</sup>; Christopher N Boddy<sup>3</sup>; Jean-Simon Diallo<sup>2,3</sup>; Jeffrey C Smith<sup>1,4</sup>; <sup>1</sup>Department of Chemistry, Carleton University, Ottawa, ON; <sup>2</sup>Centre for Cancer Therapeutics, Ottawa Hospital Research Institute, Ottawa, ON; <sup>3</sup>Department of Chemistry and Biomolecular Sciences, Ottawa, ON; <sup>4</sup>Carleton Mass Spectrometry Centre, Carleton University, Ottawa, ON
- MP 514 **In vivo oxidized neural phospholipid detection and relative quantification using GC-MS/MS and LC-MS/MS;** Secilia Garza<sup>1</sup>; Genevieve James<sup>1</sup>; Hui Gyu Park<sup>2</sup>; Paul Baker<sup>3</sup>; Mikhail Shchepinov<sup>4</sup>; J. Thomas Brenna<sup>1,2</sup>; <sup>1</sup>University of Texas, Austin, TX; <sup>2</sup>Dell Pediatric Research Institute, University of Texas at Austin, Austin, TX; <sup>3</sup>SCIEX, Redwood City, CA; <sup>4</sup>BioJiva, LLC, Los Altos, California
- MP 515 **Phospholipid compositions of human lymphoma cells revealed by LC-MS/MS utilizing trapped ion mobility spectrometry;** Dominik M Wieland<sup>1</sup>; Heiko Hayen<sup>1</sup>; <sup>1</sup>University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany
- MP 516 **A Multimodal Mass Spectrometry Approach to Profiling Sulfatides in Mouse Brains using the EAE Multiple Sclerosis Mouse Model;** Anastasiia Gordeeva<sup>1</sup>; Stephan B. Bach<sup>1</sup>; Krista Berlin<sup>1</sup>; Kayla Martinez<sup>1</sup>; <sup>1</sup>University of Texas at San Antonio, San Antonio, TX
- MP 517 **Lipidomic profiling of the ER membrane upon activation of the unfolded protein response;** Bianca De Jonckheere<sup>1,2</sup>; Paulina Kettel<sup>3,4</sup>; Elif Karagöz<sup>3,5</sup>; Robert Ahrends<sup>1</sup>; <sup>1</sup>Institute of Analytical Chemistry, University of Vienna, Vienna, Austria; <sup>2</sup>University of Vienna, Vienna Doctoral School in Chemistry, Vienna, Austria; <sup>3</sup>Max Perutz Laboratories Vienna, Vienna BioCenter, Vienna, Austria; <sup>4</sup>Vienna BioCenter PhD Program, Doctoral School of the University of Vienna and Medical University of Vienna, Vienna, Austria; <sup>5</sup>Medical University of Vienna, Vienna, Austria
- MP 518 **Dual Stable Isotope Labeling (13C, 2H) for Dynamic Lipid Analysis in Mosquito Ovaries using 21T FT-ICR MS and LC-TIMS-MS/MS;** Lilian Valadares Tose<sup>1</sup>; Janaina Isabel Mendoza Chaves<sup>1</sup>; Chad Weisbrod<sup>2</sup>; Marcela Nouzova<sup>3</sup>; Fernando Gabriel Noriega<sup>3,4,5</sup>; Francisco A Fernandez-Lima<sup>1,5</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, Florida International University, Miami, FL; <sup>2</sup>National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; <sup>3</sup>Institute of Parasitology, Biology Centre CAS, Czech Republic; <sup>4</sup>Department of Biology Sciences, Florida International University, Miami, FL; <sup>5</sup>Biomolecular Sciences Institute, Florida International University, Miami, FL
- MP 519 **Analyzing biodegradation mechanisms of benzo[a]pyrene in Pigmentiphaga kullae strain KIT-003 using GC-TQ/MS and UPLC-Q-TOF/MS;** Sung-gil Choi; <sup>1</sup>Korea Institute of Toxicology, Jinju, South Korea
- MP 520 **Application of TIMS-MRMS to the study of lipids in human blood plasma;** Viola Jeck<sup>1</sup>; Alina Theisen<sup>1</sup>; Christopher Wootton<sup>1</sup>; Matthew R Lewis<sup>2</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359, Germany; <sup>2</sup>Bruker UK Limited, Life Sciences Mass Spectrometry Division, Coventry, United Kingdom
- MP 521 **Development of an Improved Folch Method for Simultaneous Extraction of Gangliosides and Lipids from microglia-derived extracellular vesicles;** Kimberly del Carmen Molina Bean<sup>1</sup>; Shawn N. Whitehead<sup>2</sup>; Adriana Zardini Buzatto<sup>3</sup>; Shuang Zhao<sup>4</sup>; Liang Li<sup>4</sup>; <sup>1</sup>The Metabolomics Innovation Centre, Edmonton, AB; <sup>2</sup>Vulnerable Brain Laboratory, Dept. Anatomy and Cell Biology, Western University, London, Ontario; <sup>3</sup>University of Calgary, Calgary, AB; <sup>4</sup>University of Alberta, Edmonton, AB
- MP 522 **Paving the way toward analysis of Caenorhabditis elegans individuality – Development of single worm lipidomics based on nanoLC-TIMS-MS/MS;** Narayanaganesh Balasubramanian<sup>1</sup>; Klidel Fae Rellin<sup>2</sup>; Lisa Abel<sup>3</sup>; Aiko Barsh<sup>4</sup>; Sven W Meyer<sup>4</sup>; Michael Witting<sup>5</sup>; <sup>1</sup>Bruker Scientific, Fremont, CA; <sup>2</sup>Helmholtz Zentrum München German Research Center for Environmental Health, Neuherberg, Germany; <sup>3</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>4</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>5</sup>Technical University of Munich, Freising, Germany
- MP 523 **Comprehensive data acquisition workflow on Orbitrap Astral MS for untargeted lipidomics to achieve deep lipidome coverage with high confidence annotations;** Rahul Ravi Deshpande<sup>1</sup>; Ciara Myer<sup>1</sup>; Bashar Amer<sup>1</sup>; Thomas Moehring<sup>2</sup>; Susan S Bird<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

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- MP 524 **Interactions of the microbiome and radiation exposure: How may this affect emergency responses after a potential mass radiation exposure?;** Evan Pannkuk<sup>1</sup>; Igor Shuryak<sup>2</sup>; Anika Kot<sup>1</sup>; Lorreta Yun-Tien Lin<sup>1</sup>; Heng-Yong Li<sup>1</sup>; Albert J Fornace, Jr<sup>1</sup>; <sup>1</sup>Georgetown University, Washington Dc, DC; <sup>2</sup>Columbia University Irving Medical Center, New York, NY
- MP 525 **Evaluation of clustering algorithms in small molecule tandem mass spectrometry;** Xianghu Wang<sup>1</sup>; Mingxun Wang<sup>2</sup>; <sup>1</sup>University of California, Riverside, riverside, CA; <sup>2</sup>University of California, Riverside, Riverside, CA
- MP 526 **Identifying Metabolic Proliferation Mechanisms of IDH-dependent Cancer Using Liquid Chromatography-Mass Spectrometry Metabolomics;** Mathula Muhundan<sup>1</sup>; Olivia

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- Taverniti<sup>1, 2</sup>; William D. Gwynne<sup>1</sup>; Andrew T. Quail<sup>1</sup>; J. Rafael Montenegro-Burke<sup>1, 2</sup>; <sup>1</sup>Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; <sup>2</sup>Department of Molecular Genetics, University of Toronto, Toronto, ON
- MP 527 **Enabling Drug Development with Multi-Omics Integration of Host-Microbiome Crosstalk; Cristina Di Poto<sup>1</sup>; Sukithar Rajan<sup>2</sup>; Xiang Tian<sup>1</sup>; Paul Warrener<sup>3</sup>; Oliver Fiehn<sup>4</sup>; Stewart MacArthur<sup>5</sup>; Erik L. Allman<sup>1</sup>; Sonja Hess<sup>1</sup>; <sup>1</sup>Dynamic Omics, Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD; <sup>2</sup>Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Molndal, Gothenburg, Sweden; <sup>3</sup>Bacteriology, eV&I, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD; <sup>4</sup>West Coast Metabolomics Center, University of California Davis, Davis, CA; <sup>5</sup>Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Cambridge, United Kingdom**
- MP 528 **Sequential target and Non-target for Global (STANG) metabolomics in discovering prognostic biomarkers of acute ischemic stroke; Chao-Jung Chen<sup>1</sup>; Yu-Ning Lin<sup>1</sup>; <sup>1</sup>China Medical University, Taichung, Taiwan**
- MP 529 **Cell Metabolomics and Network Pharmacology: An Integrated Approach to Unravel the Potential Therapeutic Components of Astragalus radix for Allergic Rhinitis; Akshay S Patil<sup>1</sup>; Yachun Shu<sup>2</sup>; Yan Xu<sup>1</sup>; <sup>1</sup>Cleveland State university, CLEVELAND, OH; <sup>2</sup>Jiangsu Province Seaside Rehabilitation Hospital, Lianyungang, China**
- MP 530 **Metabolomics Analysis of Adherent Mammalian Cells from 96-Well Culture Plates Using Automated Sample Preparation and LC-MS/MS MRM Profiling; Edward S Folk<sup>1</sup>; Celeste Sandoval<sup>1</sup>; Sudha Gollapudi<sup>1</sup>; Christian John Ventura<sup>1</sup>; Ary Shalizi<sup>1</sup>; Phil Seitzer<sup>1</sup>; Alireza Delfarah<sup>1</sup>; Brian Feng<sup>1</sup>; Bryson Bennett<sup>1</sup>; <sup>1</sup>Calico Life Sciences, South San Francisco, CA**
- MP 531 **How does your HILIC method stack up? Optimization and comparison of common HILIC columns, mobile phases and additives for metabolomics; Sierra D. Durham<sup>1</sup>; Karen E. Yannell<sup>1</sup>; Cate Simmermaker<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA**
- MP 532 **Assessing the metabolic impact of Toxoplasmosis correlating to immune response, parasite burden and the microbiome; Caitlyn E Middleton<sup>1</sup>; Mahbobeh Lesani<sup>2</sup>; Tzu-Yu Feng<sup>3</sup>; Jan Carlos Urban Arroyo<sup>3</sup>; Eli Casarez<sup>3</sup>; Sarah Ewald<sup>3</sup>; Laura-Isobel McCall<sup>1, 4</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, San Diego State University, San Diego, CA; <sup>2</sup>Department of Microbiology and Plant Biology, University of Oklahoma, Norman, Oklahoma; <sup>3</sup>Department of Microbiology, Immunology and Cancer Biology at the Carter Immunology Center, University of Virginia School of Medicine, Charlottesville, Virginia; <sup>4</sup>Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma**
- MP 533 **Longitudinal study investigating serum metabolites and their association with type 2 diabetes risk in a Korean population; Youngae Jung<sup>1</sup>; Geum-Sook Hwang<sup>1</sup>; <sup>1</sup>Korea Basic Science Institute, Seoul, South Korea**
- MP 534 **Metabolomic Profiling of Coffea canephora Coffees: An In-Depth Exploration of Maturation Influence by UHPLC-ESI(+)-LITQ MS; Marcos V. V. Lyrio<sup>1, 2</sup>; Henzo P. Salvador<sup>3</sup>; Danieli G. Debona<sup>1</sup>; Nayara A. dos Santos<sup>2</sup>; Fábio L. Partelli<sup>3</sup>; Wanderson Romão<sup>2, 4</sup>; Eustáquio V. R. De Castro<sup>1</sup>; <sup>1</sup>Coffee Chemistry Laboratory - Coffee Design Group, Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil; <sup>2</sup>Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil; <sup>3</sup>Department of Agrarian and Biological Sciences (DCAB), University Center of Northern Espírito Santo (CEUNES), Federal University of Espírito Santo, São Mateus, Brazil; <sup>4</sup>Federal Institute of Espirito Santo, Vitória, Brazil**
- MP 535 **Increasing the detectability of phosphorylated metabolites by LC-HRMS/MS; Kathrina Mae Kumaresan<sup>1</sup>; Nathan Ghafari<sup>1</sup>; Lekha Sleno<sup>1</sup>; <sup>1</sup>University of Quebec in Montreal (UQAM), Montreal, QC**
- MP 536 **Bridging High-Coverage Metabolomics Datasets and Overcoming Batch Effect Using a Universal Metabolome Standard; Shuang Zhao<sup>1</sup>; Xiaohang Wang<sup>1</sup>; Rui Qin<sup>1</sup>; Liang Li<sup>1, 2</sup>; <sup>1</sup>The Metabolomics Innovation Centre (TMIC), Edmonton, AB; <sup>2</sup>Department of Chemistry, University of Alberta, Edmonton, AB**
- MP 537 **A system suitability scheme for assessment of longitudinal LC-TIMS-MS performance to promote reproducibility in omics sciences; Erica Marie Forsberg<sup>1</sup>; Matthew R Lewis<sup>2</sup>; Ilmari Krebs<sup>2</sup>; Patrick Groos<sup>2</sup>; Jonas Wloka<sup>2</sup>; Stefan Harsdorf<sup>2</sup>; Sven W Meyer<sup>2</sup>; <sup>1</sup>Bruker Daltonics, San Jose, CA; <sup>2</sup>Bruker Daltonics GmbH & Co. KG, Billerica, MA**
- MP 538 **Single-Point External Calibration for Quantitative Metabolomics with a Novel Microchip CE-MS Platform Coupled to HRMS; Katherine Raiche<sup>1</sup>; Sam Stewart<sup>2</sup>; Joshua P Guerrette<sup>3</sup>; Scott Mellors<sup>3</sup>; Erin Redman<sup>3</sup>; Corinne E Moss<sup>4</sup>; Katherine A Overmyer<sup>5</sup>; Joshua J Coon<sup>4</sup>; J. Will Thompson<sup>3</sup>; <sup>1</sup>908 Devices, Boston, MA; <sup>2</sup>908 Devices Inc., Boston, MA; <sup>3</sup>908 Devices Inc., Morrisville, NC; <sup>4</sup>University of Wisconsin Madison, Madison, WI; <sup>5</sup>University of Wisconsin-Madison, Madison, WI**
- MP 539 **Optimization of Analytical Methods for Metabolomics Studies of Samples Collected Using Microsampling Devices; Tiffany T Trinh<sup>1</sup>; Ruiqi Jian<sup>1</sup>; Longsha Liu<sup>1</sup>; Lihua Jiang<sup>1</sup>; Linda Lan<sup>1</sup>; Michael P. Snyder<sup>1</sup>; <sup>1</sup>Stanford University, Palo Alto, CA**
- MP 540 **Routine Targeted Metabolomic Panel Analysis from Untargeted Acquisition of Differing Mouse Plasma Populations; Cate Simmermaker<sup>1</sup>; Karen E Yannell<sup>1</sup>; Sierra D. Durham<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA**
- MP 541 **The impact of exercise on the serum proteomes and metabolomes of elite athletes participating in various sports disciplines; YOONDAM SEO; Korea Institute of Science and Technology, SEOUL, South Korea**
- MP 542 **LC-MS/MS Metabolomics of Induced Drosera capensis Digestion Reveals Broad Changes in the Abundance of Different Small Molecules; Zane G Long<sup>1</sup>; Gemma R. Takahashi<sup>2</sup>; Jonathan V. Le<sup>2</sup>; Rachel W. Martin<sup>1</sup>; <sup>1</sup>University of California, Irvine, Irvine, CA; <sup>2</sup>University of California Irvine, Irvine, CA**
- MP 543 **Macrophage Infiltration in KRAS-Driven Lung Adenocarcinoma is driven by Lipid Metabolism and TAp73 Status; Vanessa Y. Rubio<sup>1</sup>; Hayley D. Ackerman<sup>1</sup>; Nicole Hackel<sup>1</sup>; Jaden Baldwin<sup>1</sup>; John M. Koomen<sup>1</sup>; Elsa R. Flores<sup>1</sup>; <sup>1</sup>Moffitt Cancer Center, Tampa, FL**
- MP 544 **Effects of formic acid concentration and purity on chromatographic performance and ionization in untargeted metabolomics; Nathan Montgomery<sup>1</sup>; Melanie T. Odenkirk<sup>2, 3</sup>; Chi-Ming Chien<sup>2</sup>; Jacqueline Michelle Chaparro<sup>3, 4</sup>; Margaret Read<sup>3</sup>; Sarah Brinkley<sup>3, 6</sup>; Katrina L Leaprot<sup>7</sup>; Stacy D Sherrod<sup>7</sup>; Jody C May<sup>7</sup>; Cole Michel<sup>8</sup>; Katrina Doenges<sup>8</sup>; Arpana Vaniya<sup>9</sup>; John A McLean<sup>7</sup>; Richard Reisdorph<sup>8</sup>; Nichole Reisdorph<sup>8</sup>; Oliver Fiehn<sup>8</sup>; Tracy Shafizadeh<sup>2</sup>; Steve Watkins<sup>2</sup>; Jessica E Prenni<sup>3</sup>; Corey D Broeckling<sup>4</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO; <sup>2</sup>Verso Biosciences, Davis, CA; <sup>3</sup>Department of Horticulture and Landscape Architecture, Fort Collins, CO; <sup>4</sup>Analytical Resources Core: Bioanalysis and Omics Center, Colorado State University, Fort Collins, CO; <sup>5</sup>Department of Horticulture Sciences, Texas A&M University, College Station, TX; <sup>6</sup>CIAT Bioversity Alliance, Texas A&M University, College Station, TX; <sup>7</sup>Department of Chemistry and Center for Innovative Technologies, Vanderbilt University, Nashville, TN; <sup>8</sup>Skaggs School of Pharmacy and Pharmaceutical Sciences, University of Colorado, Denver,**

- CO; <sup>9</sup>West Coast Metabolomics Center, University of California Davis, Davis, CA
- MP 545 **Comprehensive Metabolomic Analysis of Human Heart Tissue and Application to Diabetic Cardiomyopathy;** Benjamin Wancewicz<sup>1</sup>; Melissa R Pergande<sup>1</sup>; Yanlong Zhu<sup>1</sup>; Zhan Gao<sup>1</sup>; Zhuoxin Shi<sup>1</sup>; Kylie Plouff<sup>1</sup>; Ying Ge<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI
- MP 546 **Multi-site metabolomic reproducibility evaluation by LC-MS;** Rebecca Jones<sup>1</sup>; Caroline Chidley<sup>2</sup>; Xiaoyang Su<sup>3</sup>; Mirela Berisa<sup>4</sup>; Drew R Jones<sup>1</sup>; Ryan D Sheldon<sup>5</sup>; <sup>1</sup>NYU Langone Health, New York, NY; <sup>2</sup>UMass Chan Medical School, Worcester, MA; <sup>3</sup>Rutgers University, New Brunswick, NJ; <sup>4</sup>Icahn School of Medicine at Mount Sinai, New York, NY; <sup>5</sup>Van Andel Institute, Grand Rapids, MI
- MP 547 **The development of a Human Metabolome Atlas uncovers metabolic signatures of hematological lineages;** Jeremy K Chan<sup>1</sup>; William D Gwynne<sup>1</sup>; Nicholas S Ly<sup>1</sup>; Brandon Y Lieng<sup>1</sup>; Olivia Taverniti<sup>1</sup>; Andrew T Quail<sup>1</sup>; J. Rafael Montenegro-Burke<sup>1</sup>; <sup>1</sup>Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON
- MP 548 **MSTUS sample-to-sample Normalization has an interesting anomaly, yielding better normalizations;** Debasish Ghosh<sup>1</sup>; Vladimir Shulaev<sup>1</sup>; Chris Beecher<sup>2</sup>; Felice de Jong<sup>3</sup>; <sup>1</sup>Department of Biological Sciences, College of Science, University of North Texas, Denton, Texas; <sup>2</sup>IROA Technologies LLC, Chapel Hill, North Carolina; <sup>3</sup>IROA Technologies LLC, Nellysford, VA
- MP 549 **Anion Exchange Chromatography Coupled with Orbitrap Mass Spectrometry for Simultaneous Quantitation and Discovery (SQUAD) Analysis of Organic Acids;** Justin Y Elliott<sup>1</sup>; Bashar Amer<sup>2</sup>; Susan S Bird<sup>2</sup>; Hussain Abdulla<sup>1</sup>; <sup>1</sup>Texas A&M Corpus Christi, Corpus Christi, TX; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- MP 550 **The influence of the microbiome on changes in the metabolome after T. cruzi infection;** Luis Ernst<sup>1</sup>; Laura-Isobel McCall<sup>1</sup>; Monica Ness<sup>2</sup>; Nathan Colwell<sup>2</sup>; Azadeh Nasuhidehnavi<sup>2</sup>; Morgan Harris<sup>2</sup>; Micah D'Armand De Chateaufvieux<sup>2</sup>; <sup>1</sup>San Diego State University, San Diego, CA; <sup>2</sup>University of Oklahoma, Norman, OK
- MP 551 **Development of a microflow metabolomics method for the detection of low-abundant metabolites;** Theodore Sana<sup>1</sup>; Rahul Deshpande<sup>2</sup>; Bashar Amer<sup>3</sup>; Susan S Bird<sup>3</sup>; Danya Dean<sup>1</sup>; Thomas Wyche<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., Cambridge, MA; <sup>2</sup>ThermoFisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific, Lexington, MA
- MP 552 **Application of Self Organizing Maps (SOM) to analyze the phenomenon of ion suppression;** Chris Beecher<sup>1</sup>; Felice A. De Jong<sup>2</sup>; Iqbal Mahmud<sup>3</sup>; Bo Wei<sup>3</sup>; Lucas Veillon<sup>3</sup>; Lin Tan<sup>3</sup>; Sara Martinez<sup>3</sup>; Bao Tran<sup>3</sup>; Alexander Raskind<sup>1</sup>; Rehan Akbani<sup>3</sup>; John N. Weinstein<sup>3</sup>; Philip L. Lorenzi<sup>3</sup>; <sup>1</sup>IROA Technologies LLC, Chapel Hill, North Carolina; <sup>2</sup>IROA Technologies LLC, Nellysford, VA; <sup>3</sup>Department of Bioinformatics and Computational Biology at The University of Texas MD Anderson, Houston, Texas
- MP 553 **Evaluation of an easily adoptable microchip CE-MS metabolomics platform to quantify hundreds of metabolites from cells and tissues;** Aurora Cabrera<sup>1</sup>; Thomas S Webb<sup>1</sup>; Scott Lyons<sup>1</sup>; Jessica Thaxton<sup>1</sup>; Saame Raza Shaikh<sup>1</sup>; Erin A. Redman<sup>2</sup>; J. Will Thompson<sup>2</sup>; Laura Herring<sup>1</sup>; <sup>1</sup>UNC-Chapel Hill, Chapel Hill, NC; <sup>2</sup>908 Devices Inc., Morrisville, NC
- MP 554 **Ion suppression correction and data normalization in metabolomics;** Iqbal Mahmud<sup>1</sup>; Bo Wei<sup>1</sup>; Lucas Veillon<sup>1</sup>; Lin Tan<sup>1</sup>; Sara Martinez<sup>1</sup>; Bao Tran<sup>1</sup>; Alexander Raskind<sup>2</sup>; Felice de Jong<sup>2</sup>; Rehan Akbani<sup>1</sup>; John N. Weinstein<sup>1</sup>; Chris Beecher<sup>2</sup>; Philip L. Lorenzi<sup>1</sup>; <sup>1</sup>MD Anderson Cancer Center, Houston, TX; <sup>2</sup>IROA Technologies LLC, Chapel Hill, NC
- MP 555 **Mass spectra annotation using learned representations in the spectrum-molecule joint embedding space;** Apurva Kalia<sup>1</sup>; Soha Hassoun<sup>1</sup>; <sup>1</sup>Tufts University, Medford, MA
- MP 556 **High-Coverage Metabolomics Analyses Identifies Ameliorative Pathway and Metabolites for Manganese-induced Parkinson's Disease Phenotype and Neurotoxicity;** Yunjia Lai<sup>1</sup>; Pablo Reina-Gonzalez<sup>2</sup>; Gali Maor<sup>3</sup>; Gary W. Miller<sup>1</sup>; Souvarish Sarkar<sup>2</sup>; <sup>1</sup>Columbia University, New York, NY; <sup>2</sup>University of Rochester, Rochester, NY; <sup>3</sup>Harvard Medical School, Boston, MA
- MP 557 **Tracing the Evolutionary Chemistry of Life through Mining of Public Metabolomics Data;** Yasin El Abiead<sup>1</sup>; Michael Strobel<sup>2</sup>; Lee R. Hagey<sup>3</sup>; Emily Gentry<sup>4</sup>; Helena Mannocho-Russo<sup>3</sup>; Paulo Wender P. Gomes<sup>3</sup>; Simone Zuffa<sup>3</sup>; Mingxun Wang<sup>2</sup>; Pieter C. Dorrestein<sup>3, 5</sup>; <sup>1</sup>Skaggs School of Pharmacy and Pharmaceutical Sciences, UCSD, San Diego, CA; <sup>2</sup>UC Riverside, Riverside, CA; <sup>3</sup>UC San Diego, La Jolla, CA; <sup>4</sup>Virginia Tech, Blacksburg, Virginia; <sup>5</sup>Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA
- MP 558 **Metabolomics assisted breeding: a new approach for the development of new crop varieties;** Amancio J De Souza<sup>1, 2</sup>; Anil Bhatia<sup>1, 2</sup>; Haiyan Ke<sup>1, 2</sup>; Manhoi Hur<sup>1, 2</sup>; Andrew Huynh<sup>1</sup>; Philip A Roberts<sup>1</sup>; Bao Lam Huynh<sup>1</sup>; <sup>1</sup>University of California Riverside, Riverside, CA; <sup>2</sup>UCR Metabolomics Core, University of California, Riverside, California
- MP 559 **GC-MS based metabolomics uncovered antioxidant pathways associated with curcumin supplementation in HepG2 induced oxidative stress;** Rossarin Tansawat<sup>1, 2</sup>; Nureesun Mahamad<sup>3</sup>; Ponsiree Jithavech<sup>1</sup>; Chawanphat Muangnoi<sup>4</sup>; <sup>1</sup>Department of Food and Pharmaceutical Chemistry, Faculty of Pharmaceutical Sciences, Chulalongkorn University, Bangkok, Thailand; <sup>2</sup>Metabolomics for Life Sciences Research Unit, Chulalongkorn University, Bangkok, Thailand; <sup>3</sup>The Halal Science Center, Chulalongkorn University, Bangkok, Thailand; <sup>4</sup>Cell and Animal Model Unit, Institute of Nutrition, Mahidol University, Nakhon Pathom, Thailand
- MP 560 **Utilization of Monodisperse Fully Porous Particles for Chromatographic Improvement in Mass Spectrometry based Metabolomics for Disease Detection;** Geoff Faden<sup>1</sup>; Timothy J. Garrett<sup>2</sup>; Ed Faden<sup>1</sup>; <sup>1</sup>MAC-MOD Analytical, Chadds Ford, PA; <sup>2</sup>University of Florida, Gainesville, FL
- MP 561 **A Dynamic Simultaneous Quantitation and Discovery (SQUAD) Liquid Chromatography Mass Spectrometry Approach for Inflammatory Bowel Disease Metabolomics in African Americans;** Jada S Gray<sup>1</sup>; Olatomiwa O Bifarin<sup>1</sup>; Samuel G. Moore<sup>1</sup>; David A. Gaul<sup>1</sup>; Sana Syed<sup>2</sup>; Adam Greene<sup>2</sup>; Jason Papin<sup>2</sup>; Gregory C Gibson<sup>1</sup>; Subra Kugathasan<sup>3</sup>; Facundo M. Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>University of Virginia, Charlottesville, VA; <sup>3</sup>Emory University School of Medicine, Atlanta, GA
- MP 562 **Evaluation of Tissues Preserved in RNAlater for Metabolomics Analysis;** Crystal L. Pace<sup>1</sup>; Bradley C. Cochran<sup>1</sup>; Richard J. Robinson<sup>1</sup>; <sup>1</sup>Metabolon Inc., Morrisville, NC
- MP 563 **Investigating metabolic consequences of cigarette smoke exposure in murine lung tissue via untargeted metabolomics and cheminformatic approaches;** Kirsten E Overdahl<sup>1</sup>; Ezazul Haque<sup>1</sup>; Darryl C. Zeldin<sup>1</sup>; Stephanie J. London<sup>1</sup>; Alan K. Jarmusch<sup>1</sup>; <sup>1</sup>National Institute of Environmental Health Sciences, Research Triangle Park, NC
- MP 564 **Performance evaluation of polarity switching for untargeted metabolomics using orbitrap mass spectrometer;** Hailemariam Abbrha Assress<sup>1, 2</sup>; Mario G. Ferruzzi<sup>1, 2</sup>; Colin D. Kay<sup>1, 2</sup>; Renny S. Lan<sup>1, 2</sup>; <sup>1</sup>Arkansas Children's Nutrition Center, Little Rock, Arkansas; <sup>2</sup>Department of Pediatrics, University of Arkansas for Medical Sciences, Little Rock, Arkansas
- MP 565 **Untargeted metabolomics workflows using correlation analysis to uncover links between metabolic pathways;**



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- Nathan Ghafari<sup>1</sup>; Lekha Sleno<sup>1</sup>; <sup>1</sup>University of Quebec in Montreal, Montreal, QC
- MP 566 **Metabolomic analysis of single-spheroids based on chemical isotope labeling micro-flow liquid chromatography-mass spectrometry**; Cyrene Catenza<sup>1</sup>; Xian Luo<sup>2</sup>; Liang Li<sup>1,2</sup>; <sup>1</sup>University of Alberta, Edmonton, AB; <sup>2</sup>The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta
- MP 567 **Using a High Performance Four-Channel CIL LC-MS Method for Discovery of Metabolites Associated with Enteric Methane Emissions in Beef Cattle**; Xiaohang Wang<sup>1</sup>; Hongwei Li<sup>2</sup>; Michael Vinsky<sup>3</sup>; Ghader Manafiazar<sup>2,4</sup>; Carolyn Fitzsimmons<sup>2,3</sup>; Liang Li<sup>5</sup>; Changxi Li<sup>2,3</sup>; <sup>1</sup>The Metabolomics Innovation Centre (TMIC), Edmonton, AB; <sup>2</sup>Department of Agricultural, University of Alberta, Edmonton, AB; <sup>3</sup>Lacombe Research and Development Centre, Agriculture and Agri-Food Canada, Lacombe, AB; <sup>4</sup>Department of Animal Science and Aquaculture, Dalhousie University, Truro, NS; <sup>5</sup>Department of Chemistry, University of Alberta, Edmonton, AB
- MP 568 **Matrix Effect Evaluation using Post-Column Infused Standards for Hydrophilic Interaction Liquid Chromatography-Mass Spectrometry Method Development**; Mengle Zhu<sup>1</sup>; Pingping Zhu<sup>1</sup>; Pascal Maas<sup>1</sup>; Lieke Lamont<sup>1</sup>; Anne-Charlotte Dubbelman<sup>1,2</sup>; Amy C. Harms<sup>1</sup>; Thomas Hankemeier<sup>1</sup>; <sup>1</sup>Metabolomics and Analytics Centre, Leiden Academic Centre of Drug Research, Leiden University, Leiden, Netherlands; <sup>2</sup>Institute of Risk Assessment Sciences, Utrecht University, Utrecht, Netherlands
- MP 569 **Characterization of metabolome and lipidome cargo of extracellular vesicles**; Khyatiben Pathak<sup>1</sup>; Caitlyn Fain<sup>1</sup>; Melissa N. Martinez<sup>1</sup>; Patrick Pirrotte<sup>1,2</sup>; <sup>1</sup>Translational Genomics Research Institute, Phoenix, AZ; <sup>2</sup>City of Hope, Duarte, CA
- MP 570 **Bioactivity-Guided Functional Metabolomics: An Integrated LC-MS/MS Microfluidics-based Bioassay Approach**; Christian Geibel<sup>1</sup>; Simon Knoblauch<sup>1</sup>; Julian Schubert<sup>1</sup>; Albert Hernandez<sup>1</sup>; Keshab Bhattarai<sup>1</sup>; Giovanni Andrea Vitale<sup>1</sup>; Paolo Stincone<sup>1</sup>; Stilianos Papadopoulos Lambidis<sup>1</sup>; Jan Straetener<sup>1</sup>; Harald Gross<sup>1</sup>; Heike Brötz-Oesterhelt<sup>1</sup>; Daniel Petras<sup>1,2</sup>; <sup>1</sup>University of Tuebingen, Germany, Tuebingen, Germany; <sup>2</sup>University of California Riverside, Riverside, CA
- MP 571 **Absolute quantitation of metabolites in murine blood plasma using machine learning: a step towards generalizing to untrained analytes**; Luke S Ferro<sup>1</sup>; Alan Wong<sup>2,3</sup>; Jack Howland<sup>1</sup>; Timothy Kassis<sup>1</sup>; Ana S.H. Costa<sup>1</sup>; Jefferson G. Pruyne<sup>1</sup>; Steven B Hooper<sup>1</sup>; Joshua D. Lauterbach<sup>1</sup>; Devesh Shah<sup>1</sup>; Mimoun Cadosch Delmar<sup>1</sup>; Jack Geremia<sup>1</sup>; Naama Kanarek<sup>2,3</sup>; Jennifer M Campbell<sup>1</sup>; <sup>1</sup>Matterworks, Somerville, MA; <sup>2</sup>Boston Children's Hospital, Boston, USA, MA; <sup>3</sup>Harvard Medical School, Boston, MA
- MP 572 **2-channels labeling and spatial distribution of metabolites in small amounts of fruits by micro-punches and LC-MS**; Vi Thanh Tran<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, AB
- MP 573 **Using lipidomics to unravel metabolic pathways in Alzheimer's disease: a follow-up study**; Mariana S Marques<sup>1,2</sup>; Leda Leme Talib<sup>3</sup>; Alessandra Sussulini<sup>1,2,4</sup>; <sup>1</sup>State University of Campinas, Campinas, Brazil; <sup>2</sup>Laboratory of Bioanalytics and Integrated Omics (LaBIOmics), University of Campinas (UNICAMP), Campinas, Brazil; <sup>3</sup>Laboratory of Neurosciences LIM27, São Paulo, Brazil; <sup>4</sup>National Institute of Science and Technology of Bioanalytics (INCTBio), University of Campinas (UNICAMP), Campinas, Brazil
- MP 574 **Untargeted metabolomics for improved detection of bisphosphonate use in equine athletes**; Bethany C Keen<sup>1,2</sup>; Fuyu Guan<sup>1,2</sup>; Mary A Robinson<sup>1,2</sup>; <sup>1</sup>Department of Clinical Studies – New Bolton Center, School of Veterinary Medicine, University of Pennsylvania, Kennett Square, PA; <sup>2</sup>Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA
- MP 575 **Two Dimensional Liquid Chromatography Tandem Mass Spectrometry Reveals Microbial Metabolites in Host-Microbe Interactions**; Stilianos Papadopoulos Lambidis<sup>1</sup>; Claudia Mirretta Barone<sup>1</sup>; Dennis Jakob<sup>1</sup>; Daniel Petras<sup>2,3</sup>; Ruth E Ley<sup>1</sup>; <sup>1</sup>Department of Microbiome Science, Max Planck Institute for Biology, Tuebingen, Germany; <sup>2</sup>University of California, Riverside, RIVERSIDE, California; <sup>3</sup>Functional Metabolomics Lab, Cluster of excellence CMFI, University of Tuebingen, Tuebingen, Germany
- MP 576 **Non-targeted profiling of Nepeta Cataria using high-dimensional gas chromatography, and high-performance mass spectrometry**; John Hayes<sup>1</sup>; David E Alonso<sup>2</sup>; Craig Fowler<sup>1</sup>; <sup>1</sup>LECO Corporation, Saint Joseph, MI; <sup>2</sup>Leco Corporation, St. Joseph, MI
- MP 577 **Machine Learning Enhanced Direct Infusion Mass Spectrometry for High-throughput Metabolomics**; Arzu Tugce Guler<sup>1</sup>; Boryana Petrova<sup>2</sup>; Tamara Hadzic<sup>3</sup>; <sup>1</sup>Institute for Experiential AI at Northeastern University, Boston, MA; <sup>2</sup>Boston Children's Hospital, Boston, MA; <sup>3</sup>Northeastern University, Boston, MA
- MP 578 **High-Throughput Screening of Bioengineered Microorganisms Using a "Fast-Pass" Desorption Electrospray Ionization-Mass Spectrometry Imaging Workflow**; Hawkins S Shepard<sup>1</sup>; Baltazar E Zuniga<sup>1</sup>; Joshua P Abraham<sup>2</sup>; Jody C May<sup>1</sup>; Brian F Pfleger<sup>2</sup>; Jamey D Young<sup>1</sup>; John A McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>University of Wisconsin-Madison, Madison, WI
- MP 579 **Exploring the Metabolome in Serum and Cerebrospinal Fluid of Traumatic Brain Injury Patients by LC-MS/MS**; Sarah A Sahioun<sup>1</sup>; Judith Nwaiwu<sup>1</sup>; Oluwatosin E Daramola<sup>1</sup>; Vishal Sandilya<sup>1</sup>; Cristian Gutierrez-Reyes<sup>1</sup>; Waziha Tasnim Purba<sup>1</sup>; Firas Kobeissy<sup>2</sup>; Stefania Mondello<sup>3</sup>; Ava M Puccio<sup>4</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, Texas; <sup>2</sup>Morehouse School of Medicine, Atlanta, Georgia; <sup>3</sup>University of Messina, Messina, Italy; <sup>4</sup>University of Pittsburgh, Pittsburgh, Pennsylvania
- MP 580 **Evaluation of automated detection of bile acid-amino acid conjugates in feces from a clinical study**; Stephen Barnes<sup>1</sup>; Landon Wilson<sup>2</sup>; Youngmee Kim<sup>3</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>University of Alabama at Birmingham, Birmingham, Alabama; <sup>3</sup>University of Miami, Miami, FL
- MP 581 **COVID-19 unevenly impacts metabolism in the periphery of the coronal plane of the lungs**; Jarrod A Roach<sup>1,2</sup>; Biyun Xue<sup>3</sup>; Jian Zheng<sup>3</sup>; Stanley Perlman<sup>3</sup>; Laura-Isobel McCall<sup>2</sup>; <sup>1</sup>University of Oklahoma, Norman, OK; <sup>2</sup>San Diego State University, San Diego, CA; <sup>3</sup>University of Iowa, Iowa City, IA
- MP 582 **An Offline Two-dimensional LC-MS Platform for Rapid Metabolome Analyses of Complex Samples**; Sicheng Quan<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, AB
- MP 583 **Achieving In-Depth Multi-omic Coverage of Exosomes through Systematic Comparison of Multiple Extractions and High-Resolution Mass Spectrometry**; Andrew J Perciaccante<sup>1</sup>; Melissa R Pergande<sup>2</sup>; Timothy J Aballo<sup>2,3</sup>; Kevin M Buck<sup>1</sup>; Ying Ge<sup>1,2,3</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, WI; <sup>2</sup>University of Wisconsin-Madison, Department of Cell and Regenerative Biology, Madison, WI; <sup>3</sup>University of Wisconsin-Madison, Molecular and Cellular Pharmacology Training Program, Madison, WI
- MP 584 **A metabolomics-guided approach for the identification of predictors of treatment response for rheumatoid arthritis**; Denise Marradi<sup>1</sup>; Camilla Dido<sup>1</sup>; Elettra Barberis<sup>2</sup>; Pier Paolo Sainaghi<sup>1</sup>; Marcello Manfredi<sup>1</sup>; <sup>1</sup>Department of Translational Medicine, University of Piemonte Orientale, Novara, Italy; <sup>2</sup>Department of Sciences and Technological Innovation, University of Piemonte Orientale, Alessandria, Italy
- MP 585 **Using molecular networking and explainable-AI to aggregate and interrogate untargeted metabolomics**

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- data for plant biology;** Manasa Appidi<sup>1</sup>; Sameer Mudbhari<sup>1</sup>; Dana L Carper<sup>2</sup>; Richard J Giannone<sup>2</sup>; Tomas Rush<sup>2</sup>; Doug Hyatt<sup>2</sup>; Daniel Jacobson<sup>2</sup>; Robert L Hettich<sup>2</sup>; Melissa Cregger<sup>2</sup>; John Field<sup>3</sup>; Udaya Kalluri<sup>2</sup>; Paul E Abraham<sup>2</sup>; <sup>1</sup>UT-ORNL Graduate School of Genome Science and Technology, University of Tennessee, Knoxville, TN, USA, Knoxville, TN; <sup>2</sup>Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; <sup>3</sup>Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
- MP 586 **Developing and Implementing a Signal Handling Approach for More Accurate Metabolite Elemental Composition Determination using Orbitraps;** Chia-Wei Hsu<sup>1</sup>; Wei-Hung Chang<sup>1</sup>; Ya-Wen Chou<sup>1</sup>; Yet-Ran Chen<sup>1</sup>; <sup>1</sup>Academia Sinica, Taipei, Taiwan
- MP 587 **Assess Poly and Perfluoroalkyl Substances (PFASs) using untargeted metabolomics in the Child Health and Development Studies;** Dongxue Wang<sup>1</sup>; Nickilou Y. Krigbaum<sup>2</sup>; Piera M. Cirillo<sup>2</sup>; ViLinh Tran<sup>3</sup>; Dean P. Jones<sup>3</sup>; Barbara A. Cohn<sup>2</sup>; Xin Hu<sup>1</sup>; <sup>1</sup>Rollins School of Public Health, Emory University, Atlanta, GA; <sup>2</sup>The Center for Research on Women and Children's Health, Public Health Institute, Berkeley, California; <sup>3</sup>School of Medicine, Emory University, Atlanta, GA
- MP 588 **A Comprehensive Study on the Regulation of Compound Zaoren Granule on Metabolic Disorder in CUMS-PCPA induced Insomnia Rats;** Yachun Shu<sup>1, 2</sup>; Zekun Wang<sup>1</sup>; Yajun Chen<sup>3</sup>; <sup>1</sup>Affiliated Hospital of Nanjing University of Chinese Medicine, Nanjing, China; <sup>2</sup>Jiangsu Province Seaside Rehabilitation Hospital, Lianyungang, China; <sup>3</sup>Nanjing Women and Children's Healthcare Hospital, Nanjing, China
- MP 589 **Empowering Research: Constructing a Comprehensive Untargeted Metabolomics Pipeline for Dynamic Microbiome Research;** Jessica C Little<sup>1, 2</sup>; Michael Mallowney<sup>1, 2</sup>; Eric Pamer<sup>1, 2</sup>; Ashley Sidebottom<sup>1, 2</sup>; <sup>1</sup>Duchossois Family Institute, Chicago, IL; <sup>2</sup>University of Chicago, Chicago, IL
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- MP 590 **Proteomic profiling to study the effect of light on Pseudomonas aeruginosa biofilms;** Lipi Das<sup>1, 2</sup>; Kelly N. Eckart<sup>1</sup>; Alexander W. Rookyard<sup>1, 2</sup>; Lars E. P. Dietrich<sup>1</sup>; Lewis M. Brown<sup>1, 2</sup>; <sup>1</sup>Department of Biological Sciences, Columbia University, New York, NY; <sup>2</sup>Quantitative Proteomics and Metabolomics Center, Columbia University, New York, NY
- MP 591 **Legacy effects of plant-soil feedbacks under drought on drought tolerance of post-succeeding soybean plants;** Yushiro Fujii<sup>1</sup>; Megumi Narukawa<sup>2</sup>; Mai Tsuda<sup>3</sup>; Yasunori Ichinashi<sup>2</sup>; Ryosuke Sasaki<sup>1</sup>; Yui Nose<sup>2</sup>; Kengo Sakurai<sup>4</sup>; Hirokazu Takahashi<sup>5</sup>; Hideki Takanashi<sup>4</sup>; Yoshihiro Omori<sup>4</sup>; Akito Kaga<sup>6</sup>; Hisashi Tsujimoto<sup>7</sup>; Mikio Nakazono<sup>5</sup>; Toru Fujiwara<sup>4</sup>; Hiroyoshi Iwata<sup>4</sup>; Masami Hirai<sup>1</sup>; <sup>1</sup>RIKEN Center for Sustainable Resource Science, Yokohama, Japan; <sup>2</sup>RIKEN BioResource Research Center, Tsukuba, Japan; <sup>3</sup>Tsukuba Univ. Tsukuba-Plant Innovation Research Center, Tsukuba, Japan; <sup>4</sup>Grad. Sch. Agr. Life Sci., Univ. Tokyo, Bunkyo-ku, Japan; <sup>5</sup>Grad. Sch. Bioagric. Sci., Nagoya Univ., Nagoya, Japan; <sup>6</sup>Inst. Crop Sci., NARO, Tsukuba, Japan; <sup>7</sup>Arid Land Res. Ctr., Tottori Univ., Tottori, Japan
- MP 592 **Lipid characterization along the zebrafish body-axis and isolated intestine using High-Resolution MALDI Imaging mass spectrometry;** Jacquelyn Spathies<sup>1</sup>; Caitlin Murdoch<sup>2, 3</sup>; Madeline E Colley<sup>4, 5</sup>; Lukasz Migas<sup>5, 6</sup>; Eric Skaar<sup>2, 3</sup>; Raf Van De Plas<sup>4, 5, 6</sup>; Jeffrey M Spraggins<sup>3, 4, 5, 7, 8</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; <sup>3</sup>Vanderbilt Institute for Infection, Immunology and Inflammation, Vanderbilt University School of Medicine, Nashville, Tennessee; <sup>4</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>5</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>6</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>7</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; <sup>8</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN
- MP 593 **Ferric Ion-based Surface-assisted Laser Desorption/Ionization Mass Spectrometry for the Analysis of Small Molecules and Microorganisms;** Tzu Ling Yang<sup>1</sup>; Chih-Wei Chen<sup>1</sup>; Yu-Chie Chen<sup>1</sup>; <sup>1</sup>National Yang Ming Chia Tung University, Hsinchu, Taiwan
- MP 594 **A binary-matrix applied in the study of bacteria;** Xinhua Guo; <sup>1</sup>Jilin University, Changchun, China
- MP 595 **Deciphering the microbiome: a targeted LC/MS/MS method for the comprehensive analysis of bile acids in biological samples;** Pietro Morlacchi<sup>1</sup>; Ruben J.F. Ramos<sup>2</sup>; Christophe Deckers<sup>3</sup>; Limian Zhao<sup>3</sup>; Mark Sartain<sup>3</sup>; Daniel Cuthbertson<sup>3</sup>; Justin R Cross<sup>2</sup>; <sup>1</sup>Agilent Technologies, Inc., Lexington, MA; <sup>2</sup>Memorial Sloan Kettering Cancer Center, New York, NY; <sup>3</sup>Agilent Technologies, Inc., Santa Clara, CA
- MP 596 **The Peptonizer2000 for taxonomic identification of metaproteomic samples with a new taxonomic quantification method;** Tanja Holstein<sup>1, 2</sup>; Pieter Verschaffelt<sup>2, 3</sup>; Lennart Martens<sup>2, 4</sup>; Thilo Muth<sup>5</sup>; <sup>1</sup>Ghent University, Ghent, Belgium; <sup>2</sup>VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; <sup>3</sup>Ghent University, Ghent, Belgium; <sup>4</sup>Gent University, Ghent, Belgium; <sup>5</sup>Robert Koch Institute, Berlin, Germany
- MP 597 **Non-invasive diagnosis of mixed invasive pulmonary aspergillosis and mucormycosis;** Dominika Luptáková<sup>1</sup>; Rutuja H. Patil<sup>2</sup>; Radim Dobiáš<sup>3</sup>; Milan Navrátil<sup>4</sup>; David A. Stevens<sup>5</sup>; Vladimír Havlíček<sup>1</sup>; <sup>1</sup>Institute of Microbiology, Prague 4, Czech Republic; <sup>2</sup>Institute of Microbiology of the Czech Academy of Sciences, 142 20, Prague, Czech Republic; <sup>3</sup>Public Health Institute, Ostrava, Czech Republic; <sup>4</sup>Department of Haematology, University Hospital Ostrava and Faculty of Medicine, University of Ostrava, Ostrava, Czech Republic; <sup>5</sup>Stanford University, Stanford, CA
- MP 598 **Proteomic characterization of a Haematococcus pluvialis (Chlorophyceae) mutant with a higher heterotrophic growth rate;** Kyarii Ramarui<sup>1</sup>; Jun Zhong<sup>2</sup>; Yantao Li<sup>1</sup>; <sup>1</sup>University of Maryland Center for Environmental Science, Institute of Marine and Environmental Technology, Baltimore, MD; <sup>2</sup>Mayo Clinic, Rochester, MN
- MP 599 **Non-targeted Metabolomics enables the Identification of Keystone Specialised Metabolites in a Phyllosphere derived Synthetic Microbial Community Model;** Paolo Stincone<sup>1, 2</sup>; Vasvi Chaudhry<sup>2</sup>; Karoline Steuer-Lodd<sup>3</sup>; Lukas Miles Braun<sup>2</sup>; Monja Schmid<sup>2</sup>; Franziska Höhn<sup>1</sup>; Nadine Ziemert<sup>1</sup>; Eric Kemen<sup>2</sup>; Daniel Petras<sup>1, 3</sup>; <sup>1</sup>University of Tuebingen, Interfaculty Institute of Microbiology and Infection Medicine, Tuebingen, Germany; <sup>2</sup>University of Tuebingen, Center for Plant Molecular Biology, Tuebingen, Germany; <sup>3</sup>University of California, Riverside, Riverside, CA
- MP 600 **Tackling the identification challenge in metaproteomics;** Tim Van Den Bossche<sup>1</sup>; Justine Lemaître<sup>1</sup>; Lennart Martens<sup>1</sup>; <sup>1</sup>VIB-UGent Center for Medical Biotechnology, VIB, Ghent, Belgium
- MP 601 **Integrative mass spectrometry based workflow to study drug resistance against aminoglycosides in Escherichia coli;** Nilanjan Ghosh Dastidar<sup>1</sup>; Nicola S. Freyer<sup>1</sup>; Ingo Wohlgemuth<sup>1</sup>; Henning Urlaub<sup>2, 3</sup>; Marina V. Rodnina<sup>1</sup>; <sup>1</sup>Department of Physical Biochemistry, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; <sup>2</sup>Bioanalytical Mass Spectrometry Group, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; <sup>3</sup>Institute of Clinical Chemistry, Bioanalytics, University Medical Center Göttingen, Göttingen, Germany
- MP 602 **Investigating the impact of different chemicals on the gut microbiota in vitro;** Vittoria F Borrini<sup>1</sup>; Denise Marradi<sup>2</sup>; Riccardo Nuzzi<sup>2</sup>; Virginia Vita Vanella<sup>2</sup>; Marco Ghirimoldi<sup>2</sup>; Beatrice Purghè<sup>2</sup>; Francesco Dondero<sup>1</sup>; Elettra Barberis<sup>1</sup>

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- MP 603 **Gut microbial metabolic pathways as opportunities for new therapeutic strategies in cardiometabolic diseases;** Ina Nemet<sup>1</sup>; Xinmin S. Li<sup>1</sup>; Arash Haghikia<sup>2, 3, 4</sup>; Lin Li<sup>1</sup>; Jennifer Wilcox<sup>1</sup>; Kymberleigh A Romano<sup>1</sup>; Jennifer A Buffa<sup>1</sup>; Marco Witkowski<sup>1</sup>; Ilija Demuth<sup>2, 5</sup>; Maximilian König<sup>2</sup>; Elisabeth Steinhagen-Thiessen<sup>2</sup>; Fredrik Bäckhed<sup>6</sup>; Michael Fischbach<sup>7, 8</sup>; W.H. Wilson Tang<sup>1, 9</sup>; Ulf Landmesser<sup>2, 3, 4</sup>; Stanley L Hazen<sup>1, 9</sup>; <sup>1</sup>Department of Cardiovascular & Metabolic Sciences and Center for Microbiome & Human Health, LRI, Cleveland Clinic, Cleveland, OH; <sup>2</sup>Charité-Universitätsmedizin, Berlin, Germany; <sup>3</sup>German Center for Cardiovascular Research, (DZHK), Germany; <sup>4</sup>Berlin Institute of Health, (BIH), Germany; <sup>5</sup>Berlin Institute of Health Center for Regenerative Therapies, Berlin, Germany; <sup>6</sup>University of Gothenburg, Gothenburg, Sweden; <sup>7</sup>ChEM-H Institute and Departments of Bioengineering and Microbiology and Immunology, Stanford University, Stanford, CA; <sup>8</sup>Chan Zuckerberg Biohub, San Francisco, CA; <sup>9</sup>Heart, Vascular, and Thoracic Institute, Cleveland Clinic, Cleveland, OH
- MP 604 **Characterization of extracellular vesicles of intestinal microbiota using metaproteomics in patients with Crohn's disease;** Celine HENRY<sup>1</sup>; Maxime Long<sup>1</sup>; Valentin Loux<sup>2</sup>; Romain Sausset<sup>1</sup>; Catherine Juste<sup>1</sup>; Marianne De Paepe<sup>1</sup>; <sup>1</sup>Université Paris-Saclay, INRAE, AgroParisTech, Micalis Institute, Jouy-en-Josas, France; <sup>2</sup>Université Paris-Saclay, INRAE, MalAGE, Jouy-en-Josas, France
- MP 605 **A metaproteome assessment of microbiome changes following microbial invasion;** Dana L Carper<sup>1</sup>; Alyssa A Carrell<sup>1</sup>; Leah H Burdick<sup>1</sup>; Dale A Pelletier<sup>1</sup>; Paul E Abraham<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN
- MP 606 **Community Curation of Microbiome Metabolites for The Mechanistic Analysis of Metabolomics Data;** Helena Mannocho-Russo<sup>1</sup>; Shipei Xing<sup>1</sup>; Fernanda De Oliveira<sup>1, 2</sup>; Wilhan D Gonçalves Nunes<sup>3</sup>; Martijn Van Faassen<sup>4</sup>; Vincent Charron-Lamoureux<sup>1</sup>; Sydney Thomas<sup>1</sup>; Paulo Wender Portal Gomes<sup>1</sup>; Marilyn De Graeve<sup>5</sup>; Haoqi Nina Zhao<sup>1</sup>; Irina Koester<sup>6</sup>; Ralph Riley Torres<sup>6</sup>; Nicole E Avalon<sup>6</sup>; Simone Zuffa<sup>1</sup>; Andrés Mauricio Caraballo-Rodríguez<sup>1</sup>; Yasin El Abiead<sup>1</sup>; Ipsita Mohanty<sup>1</sup>; Lucia Cancelada<sup>6, 7</sup>; Felipe Vasquez-Castro<sup>1</sup>; Sarolt Magyari<sup>8</sup>; Mingxun Wang<sup>9</sup>; Pieter C Dorrestein<sup>1, 10, 11, 12</sup>; <sup>1</sup>Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; <sup>2</sup>Engineering School of Lorena, University of Sao Paulo, Lorena, Brazil; <sup>3</sup>Federal Institute of Education, Science and Technology of São Paulo, Ilha Solteira, Brazil; <sup>4</sup>University Medical Center Groningen, University of Groningen, Groningen, Netherlands; <sup>5</sup>Department of Translational Physiology, Infectiology and Public Health, Ghent University, Merelbeke, Belgium; <sup>6</sup>Scripps Institution of Oceanography, University of California, San Diego, CA; <sup>7</sup>Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA; <sup>8</sup>Institute of Microbiology, ETH, Zurich, Switzerland; <sup>9</sup>Department of Computer Science, University of California Riverside, Riverside, CA; <sup>10</sup>Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; <sup>11</sup>Department of Pharmacology, University of California San Diego, La Jolla, CA; <sup>12</sup>Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA
- MP 607 **Unlocking Metaproteomics: DIA-PASEF on the timsTOF Ultra sets new depth, sensitivity, and high-throughput limits for the study of Host-Microbiome interactions;** David Gomez Varela<sup>1</sup>; Feng Xian<sup>1</sup>; Christoph Krips<sup>2</sup>; Manuela Schmidt<sup>1</sup>; <sup>1</sup>University of Vienna, Vienna, Austria; <sup>2</sup>Bruker Daltonics GmbH & Co.KG, Bremen, Germany
- MP 608 **Meta-omic analysis of anaerobic microbiomes digesting senescent switchgrass across a gradient of pH, temperature, and retention times;** Michael Shreve<sup>1</sup>; Dana L Carper<sup>2</sup>; Katharine Strandquist<sup>1</sup>; Payal Chirania<sup>3</sup>; Ikenna O Okekeogbu<sup>2</sup>; Robert L Hettich<sup>2</sup>; John M Regan<sup>1</sup>; Tom L Richard<sup>1</sup>; Richard J. Giannone<sup>2</sup>; <sup>1</sup>The Pennsylvania State University, University Park, PA; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>3</sup>The University of Tennessee Knoxville, Knoxville, TN
- MP 609 **The Solution is in Sourdough: Harnessing Microbial Diversity for Unique Chemical Composition of Bread;** Eva G Keohane<sup>1</sup>; Jacqueline M Chaparro<sup>1</sup>; Melanie Odenkirk<sup>1</sup>; Arpana Vaniya<sup>2</sup>; Josephine Wee<sup>3</sup>; Charlene Van Buiten<sup>1</sup>; Jessica E Prenni<sup>1</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO; <sup>2</sup>West Coast Metabolomics Center, University of California Davis, Davis, CA; <sup>3</sup>Pennsylvania State University, State College, Pennsylvania
- MP 610 **MALDI and DART mass spectrometry analysis of a single entity microorganism attached to a disk electrode;** Luciana V Rivera Molina<sup>1</sup>; Gabriela Campos<sup>1</sup>; Tyler C Arntz<sup>1</sup>; Aliaksei Boika<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>University of Akron, Akron, OH
- MP 611 **Targeted UHPLC-LC-MS/MS elucidates microbially derived metabolism following xanthohumol supplementation in adults with active Crohn's Disease;** Paige Jamieson<sup>1</sup>; Jan F Stevens<sup>2</sup>; Thomas O. Metz<sup>3</sup>; Ryan Bradley<sup>4</sup>; <sup>1</sup>Oregon State University, Corvallis, OR; <sup>2</sup>Oregon State University, Corvallis, Oregon; <sup>3</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>4</sup>National University of Natural Medicine, Portland, Oregon
- MP 612 **Temporal cysteine redox proteome profiling of engineered Synechococcus elongatus PCC 7942 cscB/SPS in the context of circadian disruption;** Xiaolu Li<sup>1</sup>; Pavlo Bohutskiy<sup>1</sup>; Natalie C Sadler<sup>1</sup>; Austin Gluth<sup>2</sup>; Marina A Gritsenko<sup>1</sup>; Song Feng<sup>1</sup>; Tong Zhang<sup>1</sup>; Margaret S Cheung<sup>3</sup>; Wei-Jun Qian<sup>1</sup>; <sup>1</sup>Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Washington State University, Pullman, WA; <sup>3</sup>Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA
- MP 613 **Metabolomic profiling of aromatic amino acid-derived lactic acids in fermented foods;** Megan Danielewicz<sup>1</sup>; Ryan Lieb<sup>1</sup>; Allis Chien<sup>1</sup>; Sean Spencer<sup>2</sup>; Justin L Sonnenburg<sup>2</sup>; <sup>1</sup>Stanford University Mass Spectrometry, Stanford, California; <sup>2</sup>Stanford University, Stanford, CA
- MP 614 **Impact of Sample Complexity on Measurement Dynamic Range in Microbiome Proteomics;** Megan K Elliott<sup>1, 2</sup>; Samantha L Peters<sup>2</sup>; Robert L Hettich<sup>2</sup>; Richard J Giannone<sup>2</sup>; <sup>1</sup>University of Tennessee, Knoxville, TN; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN

### NUCLEIC ACIDS AND OLIGONUCLEOTIDES I 615-640

- MP 615 **Assessment of HILIC-MS in characterizing mixtures of duplexed siRNAs;** Ming Huang<sup>1</sup>; Haibo Qiu<sup>1</sup>; Ning Li<sup>1</sup>; <sup>1</sup>Regeneron Pharmaceuticals Inc., Tarrytown, NY
- MP 616 **mRNA Oligonucleotide Characterization via Low Flow Ion Pair-Reversed Phase Chromatography and Tandem Mass Spectrometry (LF-IP-RP-MS/MS);** Roxana Eggleston-Rangel<sup>1</sup>; Jason Anspach<sup>1</sup>; Michael McGinley<sup>1</sup>; <sup>1</sup>Phenomenex, Torrance, CA
- MP 617 **From discovery to quantitative profiling of RNA modifications using template-directed RNA cleavage and bioinformatics analysis of MS2 spectra;** Anna Popova<sup>1</sup>; Xiyu Dong<sup>1</sup>; Farshad Abdollah-Nia<sup>1</sup>; Nikhil Jain<sup>2</sup>; Robert A. Britton<sup>2</sup>; James R. Williamson<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>Baylor College of Medicine, Houston, Texas
- MP 618 **From ASOs to tRNA: Comprehensive Sequence Characterization of Highly Modified Oligonucleotides by low Mathieu q resonant CID Based Dissociation Methods;** Joshua D Hinkle<sup>1</sup>; Robert L Ross<sup>2</sup>; William M McGee<sup>2</sup>; Scott Kronewitter<sup>2</sup>; Ping Yip<sup>2</sup>; John E.P. Syka<sup>1</sup>;

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- James L Stephenson Jr<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Lexington, Massachusetts
- MP 619 **Characterization of G-Quadruplexes using CID, 213 nm UVPD, and a-EPD;** Jessica G Pauling<sup>1</sup>; Jennifer S Brodbelt<sup>1</sup>; <sup>1</sup>University of Texas at Austin, Austin, TX
- MP 620 **Quantitative Proteomics Identifies Profilin-1 As A Pseudouridine-binding Protein;** Songbo Wei<sup>1</sup>; Jun Yuan<sup>2</sup>; Shiyuan Guo<sup>2</sup>; Zheng Duan<sup>1</sup>; Jernej Murn<sup>2</sup>; Yinsheng Wang<sup>2</sup>; <sup>1</sup>University of California Riverside, Riverside, CA; <sup>2</sup>University of California, Riverside, Riverside, CA
- MP 621 **The Strategies and Case studies to develop a Sensitive and Robust Bioanalytical Assays for Oligonucleotides in Rat Tissues Using LC-MS/MS;** David Zuluaga-Rave<sup>1</sup>; Leif Morin<sup>1</sup>; Aihua Liu<sup>1</sup>; <sup>1</sup>Resolian (Formerly Alliance Pharma), Malvern, PA
- MP 622 **Optimizing Sample Preparation, Chromatography, and Informatics for Improved Sequence Coverage of mRNA Therapeutics by LC/MS/MS;** Michael d Mcginley<sup>1</sup>; Roxana Eggleston-Rangel<sup>1</sup>; Alyssa Nodland<sup>1</sup>; <sup>1</sup>Phenomenex, Torrance, CA
- MP 623 **A quantitative proteomics approach for the identification of reader proteins of pseudouridine in RNA;** Andrew H Kellum Jr<sup>1</sup>; Xiaochen Liang<sup>1</sup>; Xiaochuan Liu<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- MP 624 **Development of a Microflow IPRP UHPLC-MS/MS method for improved quantitative analysis of therapeutic oligonucleotides in human plasma;** Hao Yang<sup>1</sup>; Min Du<sup>2</sup>; Neloni R. Wijeratne<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Lexington, MA
- MP 625 **Distinguishing Stereoisomers of the Cyclobutane Pyrimidine Dimer Photoproduct by Ion Mobility Mass Spectrometry and MS/MS;** Hsin-Chieh Yang<sup>1</sup>; Savannah Scruggs<sup>1</sup>; Mengqi Chai<sup>1</sup>; John-Stephen Taylor<sup>1</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University in Saint Louis, St. Louis, MO
- MP 626 **Synthesis and characterizations of oligodeoxynucleotides containing site-specifically incorporated carboxymethyl phosphotriester and assessment of their formation in DNA;** Garrit M Clabaugh<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- MP 627 **Development of a flow-through-based limited RNase T1 digestion approach for high-throughput and high sequence-coverage mapping of therapeutic mRNAs;** Shuli Tang<sup>1</sup>; Gaoyuan Liu<sup>1</sup>; Yuetian Yan<sup>1</sup>; Shunhai Wang<sup>1</sup>; Ning Li<sup>1</sup>; <sup>1</sup>Regeneron Pharmaceuticals, Tarrytown, NY
- MP 628 **High Resolution Mass Spectrometry and LC-UV Data Streams Applied to Characterizing Oligonucleotide Impurities;** Kosuke Uchiyama<sup>1</sup>; Noriko Kato<sup>1</sup>; Takeshi Nomura<sup>1</sup>; Hiroyuki Yasuda<sup>1</sup>; Simon Ashton<sup>2</sup>; Richard Price<sup>2</sup>; Helen Jose<sup>2</sup>; Neil Loftus<sup>2</sup>; Kiyoshi Kakiya<sup>3</sup>; Kazutoshi Kishi<sup>3</sup>; Yuka Fujito<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Shimadzu Corporation, Manchester, United Kingdom; <sup>3</sup>Peptistar Inc., Settsu, Japan
- MP 629 **Simultaneous Quantitation of 13 RNA Nucleotides Using Hydrophilic Interaction Chromatography Coupled With Triple Quadrupole Mass Spectrometry;** Roger E Moore<sup>1</sup>; Khyatiben Pathak<sup>2</sup>; Patrick Pirrotte<sup>1,2</sup>; <sup>1</sup>City of Hope, Duarte, CA; <sup>2</sup>Translational Genomics Research Institute, Phoenix, AZ
- MP 630 **Investigating the deamination of cytosine oxidation products in duplex DNA using isotopic labeling and LC-MS/MS;** Gabriel Robert<sup>1</sup>; Valentin Adelmard<sup>1</sup>; Guru Madugundu<sup>1</sup>; J Richard Wagner<sup>1</sup>; <sup>1</sup>Université de Sherbrooke, Sherbrooke, QC
- MP 631 **Evaluation of Rationally Designed Compounds Targeting DNA Trinucleotide Repeat Expansions by Native Mass Spectrometry;** Raihana Afroz<sup>1</sup>; Jillian Berko<sup>2</sup>; Nana A. Acheampong<sup>2</sup>; Michael K. Berko<sup>2</sup>; Aliza N. Aslam<sup>2</sup>; Sarah B. Krueger<sup>2</sup>; Varun V. Gadkari<sup>1</sup>; <sup>1</sup>University of Minnesota, Twin Cities, Minneapolis, MN; <sup>2</sup>Mount St. Mary's University, Frederick, MD
- MP 632 **Application of internal Standard MSMS quantification with oligonucleotide pharmaceuticals;** Christopher Gawlig<sup>1</sup>; Gungör Hanci<sup>1</sup>; Michael Ruehl<sup>1</sup>; <sup>1</sup>BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany
- MP 633 **Comprehensive investigation of parameters influencing oligonucleotide mass spectra following IP-RP-separation and negative polarity ionization;** Till Wehner<sup>1</sup>; Christopher Gawlig<sup>1</sup>; Michael Ruehl<sup>1</sup>; <sup>1</sup>BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany
- MP 634 **Capillary flow ion pair reversed-phase separation for very sensitive oligonucleotide LC-HRMS analysis and characterisation;** Ulrik H. Mistarz<sup>1</sup>; Shanhua Lin<sup>2</sup>; Shane L. Bechler<sup>2</sup>; Brandon H. Robson<sup>2</sup>; Ken Cook<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Allerød, Denmark; <sup>2</sup>Thermo Fisher Scientific, Sunnyvale, CA; <sup>3</sup>Thermo Fisher Scientific, Hemel Hempstead, United Kingdom
- MP 635 **Sensitive detection of post transcriptional modifications in tRNA by microflow UHPLC-HRAM-MS/MS;** Shweta Chhajed<sup>1</sup>; Robert L Ross<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Lexington, MA
- MP 636 **Metabolite Profiling of the Antisense Oligonucleotide Tofersen Using UHPLC-HRAM mass spectrometry;** Robert L Ross<sup>1</sup>; Keeley Murphy<sup>1</sup>; Stephane Houel<sup>1</sup>; Min Du<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Lexington, MA
- MP 637 **mRNA critical quality attribute analysis using a UPLC-TOF MS System and customized software;** Ying-Qing Yu<sup>1</sup>; Rebecca J. D'Esposito<sup>1</sup>; Catalin E Doneanu<sup>1</sup>; Leslie Napoletano<sup>1</sup>; Michael Zagieboylo<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- MP 638 **The Use of Chromatography, Ion Mobility, and Statistical Analyses to Characterize the Diastereomeric Composition of Phosphorothioated Oligonucleotides;** Mohsin Ali<sup>1</sup>; Sondas H. Abdelhafeez<sup>2</sup>; Ahmed M. Abdel-Megied Ali<sup>3</sup>; Michael P. Cummings<sup>2</sup>; Jace W. Jones<sup>1</sup>; <sup>1</sup>School of Pharmacy, University of Maryland, Baltimore, MD; <sup>2</sup>University of Maryland, Department of Biology, College park, MD; <sup>3</sup>School of Pharmacy, Department of Pharmaceutical Sciences, Norte Dame University of Maryland, Baltimore, MD
- MP 639 **Simplifying eukaryotic transfer RNA Modification Mapping via FPLC;** Aastha Gyawali<sup>1</sup>; Patrick A Limbach<sup>2</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH; <sup>2</sup>University of Cincinnati, Cincinnati, OH
- MP 640 **Characterization of RNA Chemical Modifications by HILIC coupled with Tandem Mass Spectrometry;** Qishan Lin<sup>1</sup>; Thomas Begley<sup>1</sup>; <sup>1</sup>University at Albany, Albany, NY

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- MP 641 **Rapid Sequencing of Peptide Mixtures using Two-Dimensional Tandem Mass Spectrometry and Graph Partitioning Algorithms;** My Phuong Le<sup>1</sup>; Yu Zhu<sup>1</sup>; David F. Gleich<sup>1</sup>; Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- MP 642 **Fragmentation pattern of double derivatized protonated peptides (H3 model peptide) by high-resolution mass spectrometry;** Leila Afiehi<sup>1,2</sup>; Benjamin Garcia<sup>3</sup>; <sup>1</sup>University of Vienna, Vienna, Austria; <sup>2</sup>Research Support Facility, Mass spectrometry unit, Vienna, Austria; <sup>3</sup>Washington University School of Medicine, St. Louis, MO
- MP 643 **Cleavable biotin-alkyne outperforms uncleavable biotin-alkyne in the identification and quantification of newly synthesized proteins;** Daniel B. McClatchy<sup>1</sup>; John R. Yates III<sup>1</sup>; <sup>1</sup>Scripps Research, La Jolla, CA
- MP 644 **Comparison of dissociation techniques for the structural characterization of GLP-1 agonists using HRMS/MS;** Rachel Dicken<sup>1</sup>; Kirk Gaston<sup>1</sup>; <sup>1</sup>US FDA, Cincinnati

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- MP 645 **Combining Microdroplet reactions with ExD fragmentation for fast characterization of proteins and antibody subunits;** Thomas E Walker<sup>1</sup>; Rachel Franklin<sup>2</sup>; Joseph Meeuswen<sup>2</sup>; Jim Lau<sup>3</sup>; <sup>1</sup>Agilent Technologies, Lexington, MA; <sup>2</sup>Agilent Technologies, Corvallis, Oregon; <sup>3</sup>Agilent Technologies, Wilmington, DE
- MP 646 **Current Role of Mass Spectrometry in Detecting Sequence Variants to facilitate Cell Line Development of Biotherapeutics;** Andrew D Mahan<sup>1</sup>; Haichuan Liu<sup>2</sup>; Zoe Zhang<sup>2</sup>; Hirsh Nanda<sup>3</sup>; <sup>1</sup>Johnson and Johnson, Spring House, PA; <sup>2</sup>SCIEX, Redwood City, CA; <sup>3</sup>Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania
- PEPTIDES: PTM IDENTIFICATION**  
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- MP 647 **TIMAHAC: Streamlined Tandem IMAC-HILIC Workflow for Simultaneous and High-Throughput Analysis of Plant Phosphoproteomics and N-glycoproteomics;** Chin-Wen Chen<sup>1</sup>; Pei-Yi Lin<sup>1</sup>; Ying-Mi Lai<sup>2</sup>; Miao-Hsia Lin<sup>3</sup>; Shu-Yu Lin<sup>4</sup>; Chuan-Chih Hsu<sup>1</sup>; <sup>1</sup>Institute of Plant and Microbial Biology, Academia Sinica, Taipei city, Taiwan; <sup>2</sup>Agricultural Biotechnology Research Center, Academia Sinica, Taipei city, Taiwan; <sup>3</sup>Department of Microbiology, National Taiwan University College of Medicine, Taipei city, Taiwan; <sup>4</sup>Academia Sinica Common Mass Spectrometry Facilities for Proteomics and Protein Modification Analysis, Academia Sinica, Taipei city, Taiwan
- MP 648 **Complimentary TIMS and ECD for Online Bottom-Up Histone Proteoform Elucidation;** Cassandra N Fuller<sup>1</sup>; Kevin Jeanne Dit Fouque<sup>1</sup>; Lilian Valadares Tose<sup>1</sup>; Francisca N De Luna Vitorino<sup>2</sup>; Benjamin A Garcia<sup>2</sup>; Francisco A Fernandez-Lima<sup>1</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, Florida International University, Miami, FL; <sup>2</sup>Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, St. Louis, MO
- MP 649 **Developing a MS-based Proteomics Approach to Study the Forms of ADP-ribosylation;** Isabel R Uribe<sup>1</sup>; Emily Zahn<sup>2</sup>; Benjamin A Garcia<sup>2</sup>; Ben Orsburn<sup>1</sup>; Anthony KL Leung<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Washington University in St. Louis, St. Louis, MO
- MP 650 **Histone Tyrosine Sulfation: Artifact or Reality?;** Menatallah M. Youssef<sup>1, 2</sup>; Miriam F. Ayad<sup>2</sup>; Lobna A. Hussein<sup>2</sup>; Maha F. Abdel-Ghany<sup>2</sup>; Kristina Hakansson<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Faculty of Pharmacy, Ain Shams University, Cairo, Egypt
- MP 651 **Temporal Phosphoproteomics Analysis of HIV-1 Reactivation from Latency;** Yennifer Delgado<sup>1, 2, 3</sup>; Sara Makanani<sup>1, 2, 3</sup>; Vivian Yang<sup>1, 2</sup>; Erin Kim<sup>1, 2</sup>; Prashant Kaushal<sup>1, 2, 3</sup>; Oliver Fregoso<sup>1, 2</sup>; Mehdi Bouhaddou<sup>1, 2, 3</sup>; <sup>1</sup>University of California, Los Angeles, Los Angeles, CA; <sup>2</sup>Department of Microbiology, Immunology, and Molecular Genetics, Los Angeles, CA; <sup>3</sup>Institute for Quantitative and Computational Biosciences, UCLA, Los Angeles, CA
- MP 652 **Global detection and quantification of viral protein post-translational modifications;** Prashant Kaushal<sup>1, 2</sup>; Mehdi Bouhaddou<sup>1, 2</sup>; <sup>1</sup>Department of Microbiology, Immunology, and Molecular Genetics, Los Angeles, CA; <sup>2</sup>Institute for Quantitative and Computational Biosciences, UCLA, Los Angeles, CA
- MP 653 **Fast disulfide mapping by integrating programmable online disulfide-ene reaction onto the bottom-up protein analysis workflow;** Keting Zhou<sup>1</sup>; Yu Xia<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China
- MP 654 **High-throughput simultaneous quantification of glycopeptides and phosphopeptides enabled by 12-plex DiLeu isobaric tags and dual-functional Ti(IV)-IMAC;** Feixuan Wu<sup>1</sup>; Danqing Wang<sup>2, 3</sup>; Dylan Nicholas T Tabang<sup>2, 4</sup>; Haiyan Lu<sup>1</sup>; Peng-Kai Liu<sup>5</sup>; Zicong Wang<sup>1</sup>; Yuan Liu<sup>1, 6</sup>; Lingjun Li<sup>1, 2</sup>; <sup>1</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>Genentech, South San Francisco, CA; <sup>4</sup>Boston Children's Hospital, Boston, USA, MA; <sup>5</sup>Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI; <sup>6</sup>Columbia University, New York, New York
- MP 655 **Differentiation of peptide epimers and its application to D-amino acid position determination using higher-energy collisional dissociation mass spectrometry;** Yuan-Chih Chen<sup>1</sup>; Hsin-Yi Wu<sup>2</sup>; Lung-Cheng Lin<sup>3</sup>; Chih-Wei Chang<sup>1</sup>; Pao-Chi Liao<sup>1</sup>; <sup>1</sup>National Cheng Kung University, Tainan, Taiwan; <sup>2</sup>National Taiwan University, Taipei City, Taiwan; <sup>3</sup>ScinoPharm Taiwan, Ltd., Tainan, Taiwan
- MP 656 **Exploring the O-Sulfation Patterns in Endogenous CCK Peptides by Trapped Ion Mobility Spectrometry;** Elena V Romanova<sup>1</sup>; Alisha Doda<sup>2</sup>; James Checco<sup>2</sup>; Jonathan Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign, Urbana, IL; <sup>2</sup>University of Nebraska - Lincoln, Lincoln, NE
- MP 657 **Differentiation of near-isobaric cysteine-modified peptides using LC-(IM)/MS/MS;** Sarah J Jones<sup>1, 2</sup>; Christopher J. Clarke<sup>1, 2</sup>; Philip J. Brownridge<sup>1, 2</sup>; Andrew R. Jones<sup>1, 3</sup>; Christoph Krisp<sup>4</sup>; Claire E. Eyers<sup>1, 2</sup>; <sup>1</sup>University of Liverpool, Liverpool, United Kingdom; <sup>2</sup>Centre for Proteome Research, Liverpool, United Kingdom; <sup>3</sup>Computational Biology Facility, Liverpool, United Kingdom; <sup>4</sup>Bruker Daltonics, Bremen, Germany
- MP 658 **Source-induced dissociation (SID) coupled to FAIMS improves higher-energy collisional dissociation (HCD)-dependent fragmentation of ADP-ribose peptides;** Taku Kasai<sup>1</sup>; Masanori Aikawa<sup>1, 2, 3</sup>; Sasha A. Singh<sup>1</sup>; <sup>1</sup>Center for Interdisciplinary Cardiovascular Sciences, Division of Cardiovascular Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA; <sup>2</sup>Center for Excellence in Vascular Biology, Cardiovascular Division, Brigham and Women's Hospital, Harvard Medical School, Boston, MA; <sup>3</sup>Channing Division of Network Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA
- MP 659 **New strategy for identification of various lipid modified PTMs from complex peptide solutions using SDC acid precipitation;** Martin R. Larsen<sup>1</sup>; Peter Toft Jensen<sup>1</sup>; Arkadiusz Nawrocki<sup>1</sup>; <sup>1</sup>Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense M, Denmark
- MP 660 **Improving the Depth and Reliability of Glycopeptide Identification Using Protein Prospector;** Peter R. Baker<sup>1</sup>; Reuben Hogan<sup>1</sup>; Robert Chalkley<sup>1</sup>; <sup>1</sup>UCSF, San Francisco, CA
- MP 661 **Systematic Robustness Testing, Linearity, Repeatability and Specificity of a Multi-attribute Method (MAM) for Biopharmaceutical Characterization and Prequalification;** Kiran Iyer; <sup>1</sup>Just Evotec Biologics, Seattle, WA
- MP 662 **N-SPyCE-enabled Delineation of Cell State-Dependent Changes to the N-terminome;** Alexandra C Turmon<sup>1</sup>; Andrew P Becker<sup>1</sup>; Alexander W Sun<sup>1</sup>; Lisa Boatner<sup>1</sup>; Nithesh Perumal<sup>1</sup>; Keriann M Backus<sup>1</sup>; <sup>1</sup>University of California Los Angeles, Los Angeles, CA
- MP 663 **Improved peptide search for identification of SUMO2/3 and ubiquitin;** Caroline Lennartsson<sup>1</sup>; Ivo A Hendriks<sup>1</sup>; Jurgen Cox<sup>2</sup>; Michael L Nielsen<sup>1</sup>; <sup>1</sup>Novo Nordisk Center for Protein Research, Copenhagen N, Denmark; <sup>2</sup>Max Planck Institute of Biochemistry, Martinsried, Germany
- MP 664 **TUPAX: Method development for the investigation of non-canonical phosphorylation;** Leonard A Daly<sup>1, 2</sup>; Christopher J. Clarke<sup>1, 2</sup>; Dominic P Byrne<sup>2</sup>; Philip J. Brownridge<sup>1, 2</sup>; Andrew J Alpert<sup>3</sup>; Patrick A Eyers<sup>2</sup>; Claire E Eyers<sup>1, 2</sup>; <sup>1</sup>Centre for Proteome Research, Liverpool, United Kingdom; <sup>2</sup>University of Liverpool, Liverpool, United Kingdom; <sup>3</sup>PolyLC Inc, Columbia, MD
- MP 665 **Peptide mapping of tryptic digests for mAbs using a novel ExD cell on the 6545XT LC/Q-TOF mass spectrometer;** Stephen Sciuto<sup>1</sup>; Maozi Liu<sup>1</sup>; Rachel Franklin<sup>2</sup>; Jerry Han<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Agilent Technologies, Corvallis, Oregon

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- MP 666 **High throughput DIA analysis of histone PTMs using ZenoTOF;** Jaison Arivalagan<sup>1</sup>; Jessica Moore<sup>1</sup>; Danielle Gutierrez<sup>1</sup>; <sup>1</sup>*Discovery Life Sciences, Huntsville, AL*
- MP 667 **A New Framework for Systematic Evaluation of Post-translational Modification Site Localization Approaches;** Pisit Wajanasara<sup>1,2,3,4</sup>; Nuno Bandeira<sup>1,2,3,4</sup>; <sup>1</sup>*University of California San Diego, La Jolla, CA*; <sup>2</sup>*Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA*; <sup>3</sup>*Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA*; <sup>4</sup>*Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*
- MP 668 **Development and optimization of mass spectrometry-based methods for site-specific identification of ADP-ribosylation;** Sara C Buch-Larsen<sup>1</sup>; Ivo A Hendriks<sup>1</sup>; Martin Rykær<sup>1</sup>; Michael L Nielsen<sup>1</sup>; <sup>1</sup>*Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen N, Denmark*
- MP 669 **Comparative Analysis of Glycoproteomic Software Tools Using a Tailored Glycan Database;** Reuben Hogan<sup>1</sup>; Robert Chalkley<sup>2</sup>; Nicholas M. Riley<sup>3</sup>; Lauren E Pepi<sup>4</sup>; Nevan Krogan<sup>2</sup>; <sup>1</sup>*University of California, San Francisco, San Francisco, CA*; <sup>2</sup>*UCSF, San Francisco, CA*; <sup>3</sup>*University of Washington, Seattle, WA*; <sup>4</sup>*Beth Israel Deaconess Medical Center, Boston, MA*
- MP 670 **Targeting Post-Translational Modifications on Herpesvirus Proteins to Eradicate Latent Infection;** Sara K. Makanani<sup>1,2</sup>; Prashant Kaushal<sup>1,2</sup>; Pu-Lin Teng<sup>3</sup>; Ting-Ting Wu<sup>3</sup>; Mehdi Bouhaddou<sup>1,2</sup>; <sup>1</sup>*Department of Microbiology, Immunology, and Molecular Genetics, UCLA, Los Angeles, CA*; <sup>2</sup>*Institute for Quantitative and Computational Biosciences, UCLA, Los Angeles, CA*; <sup>3</sup>*Department of Molecular and Medical Pharmacology, UCLA, Los Angeles, California*
- MP 671 **Untargeted characterization of substitution errors in hyper-accurate and error-prone bacterial ribosome mutant strains;** Taylor J. Lundgren<sup>1</sup>; Patricia L. Clark<sup>1</sup>; Matthew M. Champion<sup>1</sup>; <sup>1</sup>*University of Notre Dame, Notre Dame, IN*
- MP 672 **Intensity-based site localization of post-translational modifications utilizing predicted peptide fragmentation spectra;** Michael Graber<sup>1</sup>; Alexander Hogrebe<sup>1</sup>; Daniel P Zolg<sup>1</sup>; Markus Schneider<sup>1</sup>; Tobias Schmidt<sup>1</sup>; Vishal Sukumar<sup>1</sup>; Florian Seefried<sup>1</sup>; Siegfried Gessulat<sup>1</sup>; Martin Frejno<sup>1</sup>; <sup>1</sup>*MSAID, Garching, Germany*
- MP 673 **Improved Liquid Chromatography and MS/MS Methods for Sulfopeptide Identification;** Luke M Collier<sup>1</sup>; Menatallah M. Youssef<sup>1,2</sup>; Kristina Hakansson<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI*; <sup>2</sup>*Faculty of Pharmacy, Ain Shams University, Cairo, Egypt*
- PROCESS DEVELOPMENT MS**  
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- MP 674 **Mass Spectrometry evaluation of glycosylation variants and SP2/0 Host Cell Proteins during downstream processes: the case of an immunocytokine;** Ettore Gilardoni<sup>1</sup>; Lorenzo Ghezzi<sup>2</sup>; Emiliano Sani<sup>2</sup>; Riccardo Stucchi<sup>1</sup>; Dario Neri<sup>2,3</sup>; <sup>1</sup>*Philochem AG, Otelfingen, Switzerland*; <sup>2</sup>*Philigen S.p.A., Sovicille, Italy*; <sup>3</sup>*Swiss Federal Institute of Technology, Department of Chemistry and Applied Biosciences, Zurich, Switzerland*
- MP 675 **Targeted Absolute Quantification of Residual Host Cell Proteins using LC-MS/MS and Stable Isotope Labeled Peptide Standards;** Qiyao Li<sup>1</sup>; Anthony Blaszczyk<sup>1</sup>; Derrick Zhang<sup>1</sup>; Niomi R Peckham<sup>1</sup>; Zarema Kassymbek<sup>1</sup>; Jack Simpson<sup>1</sup>; <sup>1</sup>*United States Pharmacopeial Convention, Rockville, MD*
- MP 676 **A High Throughput LC-MS Method for Cell Culture Media Nutrient and Metabolite Analysis Supporting Upstream Bioprocessing;** Yun Alelyunas<sup>1</sup>; Josh Gray<sup>2</sup>; Courtney Walton<sup>1</sup>; Guillaume Bechade<sup>3</sup>; Mark Wrona<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Waters Immerse Labs, Newark, DE*; <sup>3</sup>*Waters Corporation, Wilmslow, United Kingdom*
- MP 677 **Evaluating Traditional Mass Spectrometry Against the New Generation of Emerging Analytical Technology;** Nicole A Azer<sup>1</sup>; Xin Bush<sup>1</sup>; Nicholas Trunfio<sup>1</sup>; Erica Berilla<sup>1</sup>; Casey Kohnhorst<sup>1</sup>; David Naoki Powers<sup>1</sup>; <sup>1</sup>*US Food and Drug Administration, Silver Spring, MD*
- MP 678 **Qualitative and quantitative proteomics of "high-risk" host cell proteins in monoclonal antibody bioprocessing using a novel 3M membrane technology;** Romel Dator<sup>1</sup>; Katie Stock<sup>1</sup>; Aaron Marcella<sup>1</sup>; Christine Hitomi<sup>2</sup>; Caitlin Wold<sup>2</sup>; David Chau<sup>2</sup>; Jennifer Heitkamp<sup>2</sup>; <sup>1</sup>*Materials, Life Sciences & Analytical, 3M Health Care Business Group, 3M Center, St. Paul, MN*; <sup>2</sup>*Separation and Purification Sciences Division, 3M Health Care Business Group, 3M Center, St. Paul, MN*
- MP 679 **Applying UHPLC-HRAM MS/MS/MS method to assess host cell protein clearance during the purification process development of therapeutic mAbs;** Reiko Kiyonami<sup>1</sup>; Ying Chen<sup>2</sup>; Al De Leon<sup>2</sup>; Min Du<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Lexington, MA*; <sup>2</sup>*Thermo Fisher Scientific, Bedford, MA*
- MP 680 **Characterization of spent growth media and intracellular metabolites of CHO cells using a turnkey microchip CE-HRMS based workflow;** Erin Redman<sup>1</sup>; Awab Nehala<sup>2</sup>; Stephanie R. Klaubert<sup>2</sup>; Milla Neffling<sup>2</sup>; J. Will Thompson<sup>1</sup>; <sup>1</sup>*908 Devices Inc., Morrisville, NC*; <sup>2</sup>*908 Devices Inc., Boston, MA*
- MP 681 **Optimization of a Mass Spectrometry Data Acquisition Method for Enhanced Detection of Amino Acid Misincorporations;** Nhu Q Vu<sup>1</sup>; Jun Zhang<sup>1</sup>; <sup>1</sup>*Amgen, Thousand Oaks, CA*
- MP 682 **Streamlined top-down, middle-down, and bottom-up MS characterization of biotherapeutics on a single LC-MS platform;** Ivy Kia Ngee Low<sup>1</sup>; Yee Jiun Kok<sup>1</sup>; Xuezhi Bi<sup>1,2,3</sup>; <sup>1</sup>*Bioprocessing Technology Institute, Agency for Science, Technology and Research, Singapore, Singapore*; <sup>2</sup>*Duke-NUS Medical School, Singapore, Singapore*; <sup>3</sup>*Singapore Institute of Technology, Singapore, Singapore*
- MP 683 **Understanding the Correlation between MAM and Conventional Product Quality Assays Through Multivariate Data Analysis;** Tingting Jiang<sup>1</sup>; Francis Kwofie<sup>1</sup>; Nick Attanasio<sup>1</sup>; Matthew Haas<sup>1</sup>; John Higgins<sup>1</sup>; Hari Kosanam<sup>1</sup>; <sup>1</sup>*Merck & Co., Inc., West Point, PA*
- MP 684 **Development of a streamlined cell culture metabolite profiling assay using a new nominal mass hybrid mass spectrometer;** Elsa Gorre<sup>1</sup>; Bo Zhai<sup>1</sup>; Andrew D Mahan<sup>1</sup>; Sven Hackbusch<sup>2</sup>; Cristina Jacob<sup>2</sup>; Min Du<sup>3</sup>; <sup>1</sup>*Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*Thermo Fisher Scientific, Lexington, MA*
- MP 685 **Accelerating biologic process development: Rapid Media Screening through AI/ML-Powered LC-MS Metabolomic Analysis with Universal Calibrators;** Jared Kress<sup>1</sup>; Tingting Jiang<sup>1</sup>; John Higgins<sup>1</sup>; Jack Howland<sup>2</sup>; Ana S.H. Costa<sup>2</sup>; Luke S Ferro<sup>2</sup>; Joshua D. Lauterbach<sup>2</sup>; Jefferson G. Pruyne<sup>2</sup>; Devesh Shah<sup>2</sup>; Timothy Kassis<sup>2</sup>; Jennifer M Campbell<sup>2</sup>; Hari Kosanam<sup>1</sup>; <sup>1</sup>*Merck & Co., Inc., West Point, PA*; <sup>2</sup>*Matterworks, Inc., Somerville, MA*
- PROTEINS: COMPLEXES/NON-COVALENT INTERACTIONS**  
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- MP 686 **A Novel, Proteome-based Cell Type Set Enrichment Analysis (pCtSEA);** Casimir Bamberger<sup>1</sup>; Salvador Martinez De Bartolome<sup>2</sup>; Sandra Pankow<sup>1</sup>; Jolene K. Diedrich<sup>1</sup>; Robin Park<sup>1</sup>; John R. Yates III<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, La Jolla, CA*; <sup>2</sup>*Yatiri Biosciences, San Diego, CA*
- MP 687 **Quantifying Coupled Equilibria Using Slow Mixing Mode (SLOMO) Native Mass Spectrometry;** Duong T. Bui<sup>1</sup>; Elena N. Kitova<sup>1</sup>; Lara K. Mahal<sup>1</sup>; John S. Klassen<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, AB*
- MP 688 **Determining the quaternary dynamics of small heat-shock proteins using Orbitrap charge detection-mass spectrometry;** Olav A. Johannessen<sup>1</sup>; Dominik Saman<sup>1</sup>;

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- Justin L. P. Benesch<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Oxford, Oxford, United Kingdom
- MP 689 **Mass spectrometry identification of LVV-H7 binding partners in response to alcohol dependence; Marek Smoluch<sup>1</sup>; Kinga Hartman<sup>1</sup>; Anna Drabik<sup>1</sup>; Joanna Helena Kotlinska<sup>2</sup>; Silberring Jerzy<sup>1</sup>; Przemyslaw Mielczarek<sup>1, 3</sup>; <sup>1</sup>AGH University of Krakow, Kraków, Poland; <sup>2</sup>Department of Pharmacology and Pharmacodynamics, Medical University of Lublin, Lublin, Poland; <sup>3</sup>Laboratory of Proteomics and Mass Spectrometry, Maj Institute of Pharmacology, Polish Academy of Sciences, Kraków, Poland**
- MP 690 **Exploring Interactions Between Differently Charged LL-37 Variants and Lipids by Native Mass Spectrometry; Til Erik Kundlacz<sup>1</sup>; Carla Schmidt<sup>2</sup>; <sup>1</sup>Martin Luther University Halle-Wittenberg, Halle (Saale), Germany; <sup>2</sup>Johannes Gutenberg University, Mainz, Germany**
- MP 691 **Native Mass Spectrometry Provides Insight into the Stability and Subunit Exchange Mechanism of Mutant Transthyretin Tetramers; Carter Lantz<sup>1</sup>; Robert Rider<sup>1</sup>; Sangho Yun<sup>1</sup>; David Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX**
- MP 692 **Using affinity purification mass spectrometry to interrogate TEAD protein interactions in cancer; Alissa Guarnaccia<sup>1</sup>; Philamer Calses<sup>1</sup>; Victoria Pham<sup>1</sup>; Meena Choi<sup>1</sup>; Anwesha Dey<sup>1</sup>; Jennie Lill<sup>1</sup>; <sup>1</sup>Genentech, South San Francisco, CA**
- MP 693 **Advances in UniDec Software for Biotherapeutic Characterization; Michael Thomas Marty<sup>1</sup>; Wilson Phung<sup>2</sup>; Wendy Sandoval<sup>2</sup>; <sup>1</sup>University of Arizona, Tucson, AZ; <sup>2</sup>Genentech Inc, South San Francisco, CA**
- MP 694 **Enzyme Catalysis in the Gas Phase Revealed by ES-IMS/MS; Yuen Ki Ng<sup>1</sup>; Elnaz Aliyari<sup>1</sup>; Caroline Cui<sup>1</sup>; Lars Konermann<sup>1</sup>; <sup>1</sup>The University of Western Ontario, London, ON**
- MP 695 **Synaptobrevin-2 shows a preference for negatively charged lipids; Julia Bieber<sup>1</sup>; Carla Schmidt<sup>1</sup>; <sup>1</sup>Johannes Gutenberg University, Mainz, Germany**
- MP 696 **Use of native mass spectrometry to characterize the binding of substrate and inhibitors to Salmonella FraB deglycase, a drug target; Yuan Gao<sup>1, 2</sup>; Jamison Law<sup>1, 3</sup>; Venkat Gopalan<sup>1, 3</sup>; Vicki H. Wysocki<sup>1, 2, 3</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; <sup>2</sup>Native Mass Spectrometry Guided Structural Biology Center, Ohio State University, Columbus, OH; <sup>3</sup>Center for RNA Biology, Ohio State University, Columbus, OH**
- MP 697 **LIP-MS guided drug discovery using the cancer driver Ras as a model system; Foroughsadat Absar<sup>1</sup>; Evgeniy V. Petrotchenko<sup>1</sup>; Roopa Thapar<sup>2</sup>; Edith Nagy<sup>2</sup>; Jason B. Cross<sup>2</sup>; Christoph H. Borchers<sup>1, 3, 4, 5</sup>; <sup>1</sup>Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; <sup>2</sup>M.D. Anderson Cancer Center, Institute for Applied Cancer Science, Therapeutics Discovery Division, Houston, TX; <sup>3</sup>Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; <sup>4</sup>Division of Experimental Medicine, McGill University, Montreal, QC; <sup>5</sup>Department of Pathology, McGill University, Montreal, QC**
- MP 698 **Investigating the DNA binding behaviors and inhibition for human Rad52-DNA binding domain by native mass spectrometry and surface-induced dissociation; Zihao Qi<sup>1, 2</sup>; Charles E. Bell<sup>1, 3</sup>; Vicki H. Wysocki<sup>1, 2</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; <sup>2</sup>Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH; <sup>3</sup>Department of Biological Chemistry and Pharmacology, The Ohio State University, Columbus, OH**
- MP 699 **Integrating Metabolic Glycan Phenotype Manipulation with Affinity Purification for a Systematic Exploration of Glycoprotein Interaction Networks; Xingyu Liu<sup>1</sup>; Yixuan (Axe) Xie<sup>1</sup>; Siyu Chen<sup>2</sup>; Zongtao Lin<sup>1</sup>; Sheng Ying<sup>2</sup>; Shunyang Wang<sup>2</sup>; Carlito B. Lebrilla<sup>2</sup>; Benjamin A Garcia<sup>1</sup>; <sup>1</sup>Washington University School of Medicine, St. Louis, MO; <sup>2</sup>UC Davis, Davis, CA**
- MP 700 **Unraveling the Specificity of Membrane Protein-Lipid Interactions Using Mutant Cycling and Native MS; Hiruni S Jayasekera<sup>1</sup>; Madison De Jesus<sup>1</sup>; Katherine Mae Miller<sup>1</sup>; Michael Thomas Marty<sup>1</sup>; <sup>1</sup>The University of Arizona, Tucson, AZ**
- MP 701 **Elucidating novel regulatory lncRNA-protein interactions in hematopoiesis by hybridization capture and mass spectrometry; Yuling Dai<sup>1</sup>; Isabella Whitworth<sup>1</sup>; Brian Frey<sup>1</sup>; Mabel Minji JUNG<sup>1</sup>; Jeong-Ah Kim<sup>1</sup>; Emery H. Bresnick<sup>1</sup>; Lloyd M Smith<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI**
- MP 702 **Allosteric Activation of AMP-Activated Protein Kinase Quantified using Native Mass Spectrometry; Liam Bandura<sup>1</sup>; Boris Krichel<sup>2, 3</sup>; Matther S Fisher<sup>1</sup>; Emily A Chapman<sup>1</sup>; Ying Ge<sup>1, 2, 4</sup>; <sup>1</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin; <sup>2</sup>Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>School of Life Sciences, University of Siegen, Siegen, Germany; <sup>4</sup>Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI**
- MP 703 **Systematic analysis of protein interactions using PRiSMa; Gunnar Dittmar<sup>1</sup>; Daniel Perez-Hernandez<sup>1</sup>; Sophie Rodius<sup>1</sup>; Marta Lavouras Mendes<sup>1</sup>; Mattson Jones<sup>1</sup>; <sup>1</sup>Luxembourg Institute of Health, Strassen, Luxembourg**
- MP 704 **Residue-specific mapping of the PD-1 epitope of nivolumab using X-ray footprinting mass spectrometry; Line G. Kristensen<sup>1</sup>; Yan Chen<sup>1</sup>; Christopher J. Petzold<sup>1</sup>; Sayan Gupta<sup>1</sup>; Corie Y. Ralston<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, CA**
- MP 705 **Understanding the recruitment mechanisms of peripheral membrane proteins through direct nativeMS analysis from tunable organellar-mimicking membranes; Rachel A McAllister<sup>1</sup>; Wonhyeuk Jung<sup>1</sup>; Moitrayee Bhattacharyya<sup>2</sup>; Kallol Gupta<sup>1</sup>; <sup>1</sup>Yale School of Medicine, Department of Cell Biology, New Haven, CT; <sup>2</sup>Yale School of Medicine, Department of Pharmacology, New Haven, CT**
- MP 706 **Meltome-assisted profiling of protein complexes: Prediction of protein-protein interactions by cellular thermal shift assay and its application on malaria parasites; Samuel Pazicky<sup>1</sup>; Seth Tjia<sup>1</sup>; Ka Diam Go<sup>1</sup>; Nicolas Aranciaga<sup>1</sup>; Zbynek Bozdech<sup>1</sup>; <sup>1</sup>School of Biological Sciences, Nanyang Technological University, Singapore, Singapore**
- MP 707 **Tracking Transient Protein-Protein Interactions in Targeted Protein Degradation using Proximity-Dependent Labeling Coupled to Mass Spectrometry; Shu You<sup>1</sup>; Kristina Ivanov<sup>1</sup>; Duc Tran<sup>1</sup>; Clark Peterson<sup>1</sup>; Craig Stumpf<sup>1</sup>; Alex Campos<sup>1</sup>; <sup>1</sup>Plexium, San Diego, CA**
- MP 708 **Protein Fishing for the identification of interacting proteins: Identification of novel binding partners of Bri2 BRICHOS; Helene Tigro<sup>1</sup>; Alexey Lyashkov<sup>2</sup>; Mohammed Khadeer<sup>2</sup>; Ruth Shimmo<sup>1</sup>; Luigi Ferrucci<sup>2</sup>; Janne Johansson<sup>3</sup>; Ruin Moaddel<sup>2</sup>; <sup>1</sup>Tallinn University, Tallinn, Estonia; <sup>2</sup>NIA/NIH, Baltimore, MD; <sup>3</sup>Karolinska Institutet, Solna, Sweden**
- MP 709 **Developing a computational pipeline to study dynamic cell processes under a changing proteome; Julia Kitaygorodsky<sup>1, 2</sup>; Reuben Samson<sup>1, 2</sup>; Martina Tersigni<sup>1</sup>; Payman Samavarchi-Tehrani<sup>1</sup>; Christopher Go<sup>1, 2</sup>; Queenie Hu<sup>1</sup>; William R. Hardy<sup>1</sup>; Anne-Claude Gringras<sup>1, 2</sup>; <sup>1</sup>Lunenfeld-Tanenbaum Research Institute Mount Sinai Hospital, Toronto, Ontario; <sup>2</sup>Department of Molecular Genetics, University of Toronto, Toronto, ON**
- MP 710 **Optimizing proximity proteomics on the EvoSep-timsTOF LC-MS system; Brendon Seale<sup>1</sup>; Julia Kitaygorodsky<sup>1, 2</sup>; Reuben Samson<sup>1, 2</sup>; Martina Tersigni<sup>1</sup>; Zhen-Yuan Lin<sup>1</sup>; Cassandra Wong<sup>1</sup>; Vesal Kasmaeifar<sup>1, 2</sup>;**

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- Anne-Claude Gingras<sup>1, 2</sup>; <sup>1</sup>Lunenfeld-Tanenbaum Research Institute, Toronto, ON; <sup>2</sup>University of Toronto, Toronto, ON
- MP 711 **Analysis of protein complex stability and missense protein sequence variants associated with neurodegenerative disease;** Avery M Runnebohm<sup>1</sup>; HR Sagara Wijeratne<sup>1</sup>; Whitney Smith-Kinnaman<sup>1</sup>; Emma H Doud<sup>1</sup>; Amber L Mosley<sup>1</sup>; <sup>1</sup>Indiana University School of Medicine, Indianapolis, IN
- MP 712 **Structural, Binding Site, and Functional Comparison of PCSK9 Inhibitors Discovered Utilizing a Natural Product Drug Discovery MS Platform;** Samantha J Knott<sup>1</sup>; Erik DeBloois<sup>1</sup>; Pelle Simpson<sup>1</sup>; William Old<sup>1</sup>; Marvin Yu<sup>1</sup>; Kurt Morgenstern<sup>1</sup>; Erik Zimmerman<sup>1</sup>; <sup>1</sup>Enveda Biosciences, Boulder, CO
- MP 713 **Structure and Interactions of the Endogenous Human Commander Complex;** Markku Varjosalo; *HiLIFE, University of Helsinki, Helsinki, Finland*
- MP 714 **Lactoferrin Interaction with Glycosaminoglycans studied with Native Mass Spectrometry;** Ruolan Cheng<sup>1</sup>; Daniil G. Ivanov<sup>1</sup>; Yi Du<sup>1</sup>; Igor A. Kaltashov<sup>1</sup>; <sup>1</sup>University of Massachusetts Amherst, Amherst, MA
- MP 715 **Heterogeneous Non-Canonical Inflammasome Oligomerization Probed by Narrow Quadrupole Selections and Electron Capture Charge Reduction;** Philip Lacey<sup>1</sup>; Chengliang Wang<sup>2</sup>; Jianbin Ruan<sup>2</sup>; Vicki H Wysocki<sup>1</sup>; <sup>1</sup>The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio; <sup>2</sup>The University of Connecticut Health, Farmington, Connecticut
- MP 716 **Monitoring Fe-S cluster synthesis on E. coli protein complex IscS-IscU using time-resolved native mass spectrometry;** Emily Burningham<sup>1</sup>; Shelby Oney-Hawthorne<sup>1</sup>; Cheng-Wei Lin<sup>2</sup>; David Barondeau<sup>1</sup>; David Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX; <sup>2</sup>Genentech Inc., South San Francisco, CA
- MP 717 **Experimental and Computational Methods for Increasing Coverage of Global Protein-Protein Interaction Networks in Dynamic Contexts;** Tavis J Reed<sup>1</sup>; Peter J Metzger<sup>1</sup>; Matthew D Tyl<sup>1</sup>; Alicja Tadych<sup>1</sup>; Olga G Troyanskaya<sup>1</sup>; Ileana M Cristea<sup>1</sup>; <sup>1</sup>Princeton University, Princeton, NJ
- MP 718 **The Big Break Up—Understanding Why a Subunit or Polypeptide Abandons its Noncovalent Complex;** Rachel O. Loo<sup>1</sup>; Jessie Le<sup>1</sup>; Boyu Zhao<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA
- MP 719 **Native Surface-MS/MS, Collision Induced Unfolding, and Bottom-Up Proteomics for ex-vivo spatial differentiation of endogenous cardiac using an chicken heart model;** Raul Villacob<sup>1</sup>; Sarah C Beno<sup>1</sup>; Touradj Solouki<sup>1</sup>; <sup>1</sup>Baylor University, Waco, TX
- MP 720 **Developing a Complex-centric XL-MS approach to Delineate the Human Interactome;** Sean Tang<sup>1</sup>; Clinton Yu<sup>1</sup>; Fenglong Jiao<sup>1</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>University of California-Irvine, IRVINE, CA
- MP 721 **A novel E3 technology enables efficient, effective, and economical analysis of proteomes and protein-RNA interactions;** Yanbao Yu<sup>1</sup>; Ahmed Abdelgawad<sup>1</sup>; Guotao Lu<sup>2</sup>; Gregory A Davison<sup>2</sup>; Mona Batish<sup>1</sup>; <sup>1</sup>University of Delaware, Newark, DE; <sup>2</sup>CDS Analytical LLC, Oxford, PA
- Lansing, MI; <sup>2</sup>Michigan State University Department of Chemistry, East Lansing, MI
- MP 724 **Higher dynamic range MS1 acquisition methods with parallel narrow isolation window DIA or DDA on an Orbitrap Astral mass spectrometer;** Ulises Hernandez Guzman<sup>1</sup>; Christian Thoeing<sup>2</sup>; Max Hoek<sup>2</sup>; Nicolaie Eugen Damoc<sup>2</sup>; Jesper Velgaard Olsen<sup>1</sup>; <sup>1</sup>NovoNordisk Center for Protein Research, København, Denmark; <sup>2</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- MP 725 **Accelerating Deep Proteome Sequencing with Orbitrap Astral;** John S Chlystek<sup>1</sup>; Annie Jen<sup>1</sup>; Pavel Sinitcyn<sup>2</sup>; Katherine A Overmyer<sup>1, 2, 3</sup>; Scott T Quarmby<sup>1, 3</sup>; Joshua J Coon<sup>1, 2, 3, 4</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Biomolecular Chemistry, Madison, WI; <sup>2</sup>Morgridge Institute for Research, Madison, WI; <sup>3</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI; <sup>4</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin
- MP 726 **Connecting the Dots: A Closer Look at Cleavage Preferences of Proline Semi-Specific Endopeptidases;** Zuzana Kalaninova<sup>1, 2</sup>; Jasmina M Portasikova<sup>1, 2</sup>; Barbora Jireckova<sup>1, 2</sup>; Daniel Kavan<sup>1, 2</sup>; Jana Novakova<sup>3</sup>; Tibor Mosko<sup>4</sup>; Karel Holada<sup>4</sup>; Petr Pompach<sup>5</sup>; Petr Novak<sup>1, 2</sup>; Petr Man<sup>1, 2</sup>; <sup>1</sup>Faculty of Science, Charles University, Prague, Czech Republic; <sup>2</sup>BioCev – Institute of Microbiology, The Czech Academy of Sciences, Prague, Czech Republic; <sup>3</sup>AffiPro s.r.o, Vestec, Czech Republic; <sup>4</sup>Institute of Immunology and Microbiology, 1st Faculty of Medicine, Charles University, Prague, Czech Republic; <sup>5</sup>BioCev – Institute of Biotechnology, The Czech Academy of Sciences, Prague, Czech Republic
- MP 727 **Deep learning models combined to ultrafast DIA analysis enables rapid pathogen identification in urinary tract infections;** Florence Roux-Dalvai<sup>1</sup>; Antoine Lacombe-Rastoll<sup>1</sup>; Simon Pelletier<sup>1</sup>; Clarisse Gotti<sup>1</sup>; Mickaël Leclercq<sup>1</sup>; Ève Bérubé<sup>2</sup>; Marie-Ève Thibeault<sup>1</sup>; Maurice Boissinot<sup>2</sup>; Cristina C. Jacob<sup>3</sup>; Neloni R. Wijeratne<sup>3</sup>; Dorte B. Bekker-Jensen<sup>4</sup>; Nicolai Bache<sup>4</sup>; Maciej Bromirski<sup>5</sup>; Sandra Isabel<sup>2</sup>; Arnaud Droit<sup>1</sup>; <sup>1</sup>AD Lab - Proteomics and Computational Biology laboratory, CHU de Québec - Université Laval Research Center, Québec, QC; <sup>2</sup>Infectiology Research Centre, CHU de Québec Université Laval Research Center, Québec, QC; <sup>3</sup>ThermoFisher Scientific, San Jose, CA; <sup>4</sup>Evosep, Odense, Denmark; <sup>5</sup>Thermo Fisher Scientific, Bremen, Germany
- MP 728 **Enhanced secretomics workflow reveals organ-dependent secreted protein landscape across multiple murine tissues;** Amanda L Smythers<sup>1, 2</sup>; Joao A. Paulo<sup>1</sup>; Melanie J Mittenbuhler<sup>1, 2</sup>; Katherine A Blackmore<sup>1, 2</sup>; Sumeet A Khetarpal<sup>2, 3</sup>; Bruce M Spiegelman<sup>1, 2</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup>Harvard Medical School, Boston, MA; <sup>2</sup>Dana Farber Cancer Institute, Boston, USA, MA; <sup>3</sup>Massachusetts General Hospital, Harvard Medical School, Charlestown, MA
- MP 729 **Enhancing Sensitivity in Single-Cell Proteomics: Upgrading Triple Quadrupole Mass Spectrometer with S-Funnel Interface for Precise Quantitative Analysis;** Sehong Min<sup>1</sup>; Pearl Kwantwi-Barima<sup>1</sup>; Isaac K. Attah<sup>1</sup>; Thomas L. Fillmore<sup>2</sup>; Matthew J. Gaffrey<sup>1</sup>; William B. Chrisler<sup>1</sup>; Reta Birhanu Kitata<sup>1</sup>; Yehia M. Ibrahim<sup>1</sup>; Tujin Shi<sup>1</sup>; <sup>1</sup>Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA
- MP 730 **Ever Simpler: Streamlining Proteomics with S-Trap Turbo and BCA-No-More;** Stefan Loroch<sup>1, 2</sup>; Sandra Wilson<sup>1</sup>; Alexandre Zougman<sup>3</sup>; John P Wilson<sup>1</sup>; <sup>1</sup>Protifi, LLC, Fairport, NY; <sup>2</sup>Ruhr-University Bochum, Bochum, Germany; <sup>3</sup>University of Leeds, Leeds, United Kingdom
- MP 731 **Highly multiplexed proximity labeling proteomics for spatiotemporal profiling of the suborganellar proteome;** Dong-Gi Jang<sup>1, 2</sup>; Sanghee Shin<sup>1, 2</sup>; Song-Yi Lee<sup>3</sup>; Yeon Choi<sup>2</sup>; Hyun-Woo Rhee<sup>3</sup>; Jong-Seo Kim<sup>1, 2</sup>; <sup>1</sup>School of

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- MP 722 **Optimizing Digestion Efficiency: Impact of Various Denaturing Reagents on a 60-Biomarker Health Surveillance Panel in Human Plasma;** Erika Hernandez<sup>1</sup>; Dragana Noe<sup>1</sup>; Nathan Hendricks<sup>1</sup>; Susan M. Mockus<sup>1</sup>; <sup>1</sup>Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA
- MP 723 **A Rapid, Reproducible, and Automated cIEF-ESI-MS Method for High-Throughput Top-Down Proteomic Analysis of Nanoparticle Protein Corona;** Reyhane Tabatabaieian Nimavard<sup>1</sup>; Guijie Zhu<sup>2</sup>; Amirhossein Sadeghi<sup>2</sup>; Liangliang Sun<sup>2</sup>; <sup>1</sup>Michigan State University, -East



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- Biological Sciences, Seoul National University, Seoul, South Korea; <sup>2</sup>Center for RNA Research, Institute of Basic Science (IBS), Seoul, South Korea; <sup>3</sup>Department of Chemistry, Seoul National University, Seoul, South Korea
- MP 732 **Integrated sequencing of transcripts and proteins at the single molecule level to detect isoforms and proteotypic peptides in filament biomarkers;** Kenneth A. Skinner<sup>1</sup>; Natchanon Sittipongpittaya<sup>2</sup>; Gloria Sheynkman<sup>2</sup>; <sup>1</sup>Quantum-Si Incorporated, Branford, CT; <sup>2</sup>University of Virginia, Charlottesville, VA
- MP 733 **Nanosecond infrared laser (NIRL) based tissue sampling enables spatially resolved proteomics for identification of region-specific metabolic processes in renal tissue;** Manuela Moritz<sup>1</sup>; Annika Gerdes<sup>1</sup>; Antonia Gocke<sup>1</sup>; Hartmut Schlüter<sup>1</sup>; Jan Hahn<sup>1</sup>; <sup>1</sup>University Medical Center Hamburg-Eppendorf (UKE), Hamburg, Germany
- MP 734 **Protein cooking: gas phase separation of protein fragment ions generated by Thermal-CID;** Hieu Cuong Le<sup>1</sup>; Patrick Pribil<sup>1</sup>; Yves Le Blanc<sup>2</sup>; <sup>1</sup>SCIEX, Concord, ON; <sup>2</sup>SCIEX, Concord, ON, ON
- MP 735 **Proteomics method development for systems-wide protein turnover measurements in cynomolgus monkey;** Ghazaleh Yassaghi<sup>1</sup>; Vahid Farrokhi<sup>1</sup>; Hendrik Neubert<sup>1</sup>; <sup>1</sup>Pfizer Inc., Andover, MA
- MP 736 **Reagent restoration using crosslinking chemistry improves BioID data quality;** Jonathan St-Germain<sup>1</sup>; Faith Au Yeung<sup>2</sup>; Vinitha Macwan<sup>2</sup>; Brian Raught<sup>2</sup>; <sup>1</sup>Princess Margaret Cancer Centre, Toronto, ON; <sup>2</sup>Princess Margaret Cancer Centre, University Health Network, Toronto, ON
- MP 737 **Targeting the small proteome: Specialized methods for sequencing and the discovery of small proteins / sORFs in prokaryotes;** Jakob Meier-Credo<sup>1</sup>; Benjamin Heiniger<sup>2</sup>; Christian H. Ahrens<sup>2</sup>; Julian D. Langer<sup>1, 3</sup>; <sup>1</sup>Max-Planck-Institute of Biophysics, Frankfurt, Germany; <sup>2</sup>Molecular Ecology, Agroscope & SIB Swiss Institute of Bioinformatics, Zurich, Switzerland; <sup>3</sup>Max Planck Institute for Brain Research, Frankfurt, Germany
- MP 738 **Throughput and the Plasma Proteome- How Olink and LCMS can Synergize Biomarker Discovery;** Jessica Moore<sup>1</sup>; Jaison Arivalagan<sup>1</sup>; Tiffany Louie<sup>1</sup>; Ray Clemens<sup>1</sup>; Leslie Wilkinson<sup>1</sup>; Ana Gil De Bona<sup>1</sup>; Danielle Gutierrez<sup>1</sup>; <sup>1</sup>Discovery Life Sciences, Huntsville, AL
- MP 739 **Towards proteome analysis of single extracellular vesicles;** Ole Østergaard<sup>1</sup>; Pierre Sabatier<sup>1, 2</sup>; Charlotte Hjort<sup>1</sup>; Jesper Velgaard Olsen<sup>1</sup>; <sup>1</sup>NNF CENTER FOR PROTEIN RESEARCH, Copenhagen, Denmark; <sup>2</sup>Department of Surgical Sciences, Uppsala University, Uppsala, Sweden
- MP 740 **A Novel Proteomics Magnetic Clean-up Bead for Automated Mass Spectrometry Sample Preparation;** Maowei Dou<sup>1</sup>; Suzanne Smith<sup>1</sup>; Erum Raja<sup>1</sup>; Leigh Foster<sup>1</sup>; Kevin Yang<sup>2</sup>; Amiransoor Hakim<sup>2</sup>; Kay Opperman<sup>1</sup>; Bhavin Patel<sup>1</sup>; Ryan Bomgarden<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Rockford, Illinois; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- MP 741 **Direct Identification of Intact Proteins Using a Low-Resolution Mass Spectrometer with CIDn/ETnoD;** Cheng-Yu Kuo<sup>1</sup>; Jie-Teng Toh<sup>1</sup>; Yi-Feng Zheng<sup>1</sup>; Wei-Chen Wang<sup>1</sup>; Han-ju Chien<sup>2</sup>; Chien-Chen Lai<sup>1, 3, 4, 5, 6</sup>; <sup>1</sup>Institute of Molecular Biology, National Chung Hsing University, Taichung city, Taiwan; <sup>2</sup>Department of Biochemical Science and Technology, National Chiayi University, Chiayi city, Taiwan; <sup>3</sup>Advanced Plant Biotechnology Center, National Chung Hsing University, Taichung city, Taiwan; <sup>4</sup>Graduate Institute of Chinese Medical Science, China Medical University, Taichung city, Taiwan; <sup>5</sup>Ph.D. Program in Translational Medicine, National Chung Hsing University, Taichung, Taiwan; <sup>6</sup>Rong Hsing Research Center for Translational Medicine, National Chung Hsing University, Taichung, Taiwan
- MP 742 **Studying the Proteome Heterogeneity of Naïve Human Pluripotent Stem Cells and Trophectoderm-like Cells Using Label-free Single-cell Proteomics;** Julia Bubis<sup>1</sup>; Harunobu Kagawa<sup>2</sup>; Manuel Matzinger<sup>1</sup>; Jana Slovakova<sup>2</sup>; Theresa M. Sommer<sup>2</sup>; Tabiwang N Arrey<sup>3</sup>; Eugen Damoc<sup>3</sup>; Peter Pichler<sup>1</sup>; Nicolas Rivron<sup>2</sup>; Karl Mechtler<sup>1</sup>; <sup>1</sup>Research Institute of Molecular Pathology (IMP), Vienna BioCenter, Vienna, Austria; <sup>2</sup>Institute of Molecular Biotechnology (IMBA), Austrian Academy of Sciences, Vienna BioCenter (VBC), Vienna, Austria; <sup>3</sup>Thermo Fisher Scientific, Bremen, Germany
- MP 743 **Differential ion mobility on an Astral mass spectrometer provides new insights into thymocyte maturation;** Eric Bonneil<sup>1</sup>; Sylvie Brochu<sup>1</sup>; Lilian Heil<sup>2</sup>; Tonya Pekar-Hart<sup>2</sup>; Michael W. Belford<sup>3</sup>; Cornelia Boeser<sup>3</sup>; Jean-Jacques Dunyach<sup>3</sup>; Claude Perreault<sup>4, 5</sup>; Pierre Thibault<sup>4, 6</sup>; <sup>1</sup>Université de Montreal, Montreal, QC; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>ThermoFisher Scientific, San Jose, CA; <sup>4</sup>IRIC Université de Montréal, Montreal, QC; <sup>5</sup>Department of Medicine, Université de Montréal, Montreal, QC; <sup>6</sup>Department Of Chemistry Université de Montréal, Montreal, QC
- MP 744 **Optimization of data-dependent acquisition settings for TMT-based single-cell proteome profiling;** Sachini N Moratuwage<sup>1</sup>; Kei Webber<sup>1</sup>; Xiaofeng Xie<sup>1</sup>; Siqi Huang<sup>1</sup>; Nathaniel Axtell<sup>1</sup>; Ryan T. Kelly<sup>1</sup>; <sup>1</sup>Brigham Young University, Provo, UT
- MP 745 **MALDI-ICC and SpaceM on PBMCs Spiked with Cancer Cells for Highly Multiplexed, Multiomic and Multimodal Single-Cell Profiling;** Ziyang Liu<sup>1</sup>; Gargey Yagnik<sup>1</sup>; Sharath K. Menon<sup>2</sup>; Shawn Owens<sup>3</sup>; Leonardo G. Dettori<sup>1</sup>; Philip Carvalho<sup>1</sup>; Kenneth J. Rothschild<sup>1, 4</sup>; Theodore Alexandrov<sup>2, 3, 5</sup>; Mark J. Lim<sup>1</sup>; <sup>1</sup>AmberGen Inc., Billerica, MA; <sup>2</sup>Structural and Computational Biology Unit, European Molecular Biology Laboratory (EMBL), Heidelberg, Germany; <sup>3</sup>BioStudio, BiolInnovation Institute, Copenhagen, Denmark; <sup>4</sup>Department of Physics and Photonics Center, Boston University, Boston, MA; <sup>5</sup>Molecular Medicine Partnership Unit, EMBL and Heidelberg University, Heidelberg, Germany
- MP 746 **scPiMS: a novel strategy for profiling intact proteoform signals from single cells;** Jared Kafader<sup>1</sup>; Pei Su<sup>1</sup>; Michael A. Hollas<sup>1</sup>; Stanislav Rubakhin<sup>2</sup>; Ryan T. Fellers<sup>1</sup>; Jonathan V Sweedler<sup>2</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>University of Illinois at Urbana-Champaign, Champaign, Illinois
- MP 747 **Robust, convenient, high throughput single cell proteomics;** Reta Birhanu Kitata<sup>1</sup>; Zhangyang Xu<sup>1</sup>; Rui Zhao<sup>2</sup>; Daniel J. Orton<sup>1</sup>; Nadia Bayou<sup>3</sup>; Mara Serena Serafini<sup>3</sup>; Thomas L. Fillmore<sup>2</sup>; William B. Chrisler<sup>1</sup>; Matthew J. Gaffrey<sup>1</sup>; Tao Liu<sup>1</sup>; Carolina Reduzzi<sup>3</sup>; Tujin Shi<sup>1</sup>; <sup>1</sup>Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; <sup>3</sup>Division of Hematology and Medical Oncology, Department of Medicine, Weill Cornell School of Medicine, New York, NY
- MP 748 **High-Throughput Single-Cell Metabolomics with SpaceM: High Reproducibility Enables Studying Multiple Cell Types;** Jeany Delafiori<sup>1</sup>; Shahraz Mohammed<sup>1</sup>; Andreas Eisenbarth<sup>1</sup>; Bishoy Wadie<sup>1</sup>; Bernhard Drotleff<sup>1</sup>; Mans Ekelof<sup>1</sup>; Alexander Mattausch<sup>1</sup>; Volker Hilsenstein<sup>1</sup>; Theodore Alexandrov<sup>1</sup>; <sup>1</sup>EMBL, Heidelberg, Germany
- MP 749 **Statistical methods for handling cellular heterogeneity in quantitative scMS experiments: review simulations and recommendations;** Hannah Boekweg<sup>1</sup>; Devon Kohler<sup>2</sup>; Samuel H Payne<sup>3</sup>; Olga Vitek<sup>2</sup>; <sup>1</sup>Brigham Young University, Provo, UT; <sup>2</sup>Northeastern University, Boston, MA; <sup>3</sup>BYU, Provo, UT
- MP 750 **Label-free capillary electrophoresis-mass spectrometry to study native N-glycome of single mammalian cells and ng-level blood isolates;** Anne-Lise Marie<sup>1</sup>; Yunfan Gao<sup>1</sup>; Alexander R. Ivanov<sup>1</sup>; <sup>1</sup>Barnett Institute of Chemical and

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- MP 751 **Biological Analysis, Dept. of Chemistry and Chemical Biology, Northeastern University, Boston, MA**  
**Label-free DIA-based workflow for single cell proteomic analysis using Evosep One and the Orbitrap Astral mass spectrometer;** Fernanda Salvato<sup>1</sup>; Min Huang<sup>2</sup>; Bernard Delanghe<sup>3</sup>; Kevin Yang<sup>1</sup>; Xiangjun Li<sup>4</sup>; Dorte-Bekker Jensen<sup>5</sup>; Nicolai Bache<sup>5</sup>; Tonya Pekar Hart<sup>1</sup>; Amirmansoor Hakimi<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>ThermoFisher Scientific, Shanghai, China; <sup>3</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; <sup>4</sup>Thermo Fisher Scientific, Shanghai, China; <sup>5</sup>Evosep, Odense, Denmark
- MP 752 **Label-free DIA-based workflow for single-cell proteomic analysis on an Orbitrap Exploris 480 mass spectrometer.;** Fernanda Salvato<sup>1</sup>; Bernard Delanghe<sup>2</sup>; Julia Kraegenbring<sup>2</sup>; David Hartlmayr<sup>3</sup>; Anjali Seth<sup>3</sup>; Tonya Pekar Hart<sup>4</sup>; Amirmansoor Hakimi<sup>5</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific GmbH, Bremen, Germany; <sup>3</sup>Cellenion, Lyon, France; <sup>4</sup>Thermo Fisher Scientific – 355 River Oaks Pkwy, San Jose, California; <sup>5</sup>ThermoFisher Scientific, San Jose, CA
- MP 753 **Single Cell Fatty Acid Profiling with C=C Specificity using Multiple Reaction Monitoring(MRM)-profiling and Charge Switch Derivatization;** Pooja Saklani<sup>1</sup>; Caitlin Randolph<sup>2</sup>; Brianna Corman<sup>3</sup>; Gaurav Chopra<sup>2, 4, 5, 6, 7, 8, 9</sup>; <sup>1</sup>Purdue University Department of Chemistry, West Lafayette, IN; <sup>2</sup>Purdue University, Department of Chemistry, West Lafayette, IN; <sup>3</sup>Department of Comparative Pathobiology, Purdue University, West Lafayette, IN; <sup>4</sup>Department of Computer Science (by courtesy), Purdue University, West Lafayette, IN; <sup>5</sup>Purdue Institute for Drug Discovery, West Lafayette, IN; <sup>6</sup>Regenstrief Center for Healthcare Engineering, West Lafayette, IN; <sup>7</sup>Purdue Institute for Cancer Research, West Lafayette, IN; <sup>8</sup>Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; <sup>9</sup>Purdue Institute for Integrative Neuroscience, West Lafayette, IN
- MP 754 **Dynamics of single-cell protein covariation during epithelial-mesenchymal transition;** Saad Khan<sup>1</sup>; Rachel Conover<sup>1</sup>; Anand Asthagiri<sup>1</sup>; Nikolai Slavov<sup>1, 2</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Parallel Squared Technology Institute, Watertown, MA
- MP 755 **Increasing throughput while maintaining coverage depths in single cell proteomics using the timsTOF Ultra;** Christoph Krisp<sup>1</sup>; David Hartlmayr<sup>2</sup>; Anjali Seth<sup>2</sup>; Guilhem Tourniaire<sup>2</sup>; Taylor Skurnac<sup>3</sup>; Thorsten Ledertheil<sup>1</sup>; Jean-François Greisch<sup>4</sup>; Markus Lubeck<sup>1</sup>; Liling Fang<sup>5</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co.KG, Bremen, Germany; <sup>2</sup>Cellenion, Lyon, France; <sup>3</sup>Bruker Scientific, Billerica, MA; <sup>4</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>5</sup>Bruker Scientific LLC, Billerica, MA
- MP 756 **Furthering Capabilities in Single Cell Metabolomics Using Single Cell Printing-Liquid Vortex Capture-Mass Spectrometry;** Stephen C Zambrzycki<sup>1</sup>; Vilmos Kertesz<sup>1</sup>; John F. Cahill<sup>1</sup>; <sup>1</sup>Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
- MP 757 **A Microfluidic Platform for Extracellular Vesicle Sorting and Inline ESI-MS Analysis for Cell Therapy Biomanufacturing;** Gianna A Slusher<sup>1</sup>; Peter Kottke<sup>1</sup>; Andrei Fedorov<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA
- MP 758 **Single-cell MS lipid analysis: sample storage;** Stanislav Rubakhin<sup>1, 2</sup>; Jonathan V Sweedler<sup>1, 2</sup>; <sup>1</sup>The Chemistry Department, University of Illinois at Urbana-Champaign, Urbana, IL; <sup>2</sup>Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, IL
- MP 759 **Tame Your Metabolomics Data Analysis with MeDUSA;** Laura A Hetzel<sup>1</sup>; Eric Hetzel<sup>1</sup>; Thomas Hankemeier<sup>1</sup>; Ahmed Ali<sup>1</sup>; <sup>1</sup>Universiteit Leiden, Leiden, Netherlands
- MP 760 **Systematic evaluation of proteomics variation in label-free and multiplex single-cell proteomics workflows;** Ritin Sharma<sup>1, 2</sup>; Krystine Garcia-Mansfield<sup>1, 2</sup>; Brooke Lovell<sup>1</sup>; Rochelle Kofman<sup>1</sup>; Melissa N Martinez<sup>1, 2</sup>; Joshua Cantlon<sup>3</sup>; Andrew Leduc<sup>4</sup>; Patrick Pirrotte<sup>1, 2</sup>; <sup>1</sup>Cancer and Cell Biology, Translational Genomics Research Institute, Phoenix, AZ; <sup>2</sup>Integrated Mass Spectrometry Shared Resource, City of Hope Comprehensive Cancer Center, Duarte, CA; <sup>3</sup>SCIENION US Inc., Phoenix, AZ; <sup>4</sup>Departments of Bioengineering, Biology, Chemistry and Chemical Biology, Single Cell Proteomics Center, and Barnett Institute, Northeastern University, Boston, MA
- MP 761 **Proteome asymmetry in mouse and human embryos before fate specification;** Aleksandra Petelski; Parallel Squared Technology Institute, Watertown, MA
- MP 762 **Non-small cell Lung cancer single spheroid analysis using the cellenONE with proteoCHIP EVO 96 workflow on the timsTOF Ultra;** Christoph Krisp<sup>1</sup>; Verena Tellstroem<sup>1</sup>; David Hartlmayr<sup>2</sup>; Anjali Seth<sup>2</sup>; Guilhem Tourniaire<sup>2</sup>; Dorte Bekker-Jensen<sup>3</sup>; Nicolai Bache<sup>3</sup>; Markus Lubeck<sup>1</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co.KG, Bremen, Germany; <sup>2</sup>Cellenion, Lyon, France; <sup>3</sup>Evosep, Odense, Denmark
- MP 763 **Development of rapid and accurate cell picking and semi-automatic pretreatment system for single-cell proteomic and metabolomic analysis;** Kosuke Hata<sup>1</sup>; Masatomo Takahashi<sup>1</sup>; Mamoru Hirafuji<sup>2</sup>; Keisuke Nakata<sup>1</sup>; Kazuki Ikeda<sup>1</sup>; Maiko Goto<sup>1</sup>; Mie Uetsu<sup>1</sup>; Takeshi Bamba<sup>1</sup>; Yoshihiro Izumi<sup>1</sup>; <sup>1</sup>Medical Institute of Bioregulation, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka-shi, Japan; <sup>2</sup>YODAKA Co., Ltd., 7-7 Shinkawasaki, Saiwai-ku, Kawasaki-shi, Japan
- MP 764 **Lie to me – The Importance of Knowing the Single Cell Proteomics Background;** Rupert Laurenz Mayer<sup>1</sup>; Julia A Bubis<sup>1</sup>; Manuel Matzinger<sup>1</sup>; Karl Mechtler<sup>1, 2, 3</sup>; <sup>1</sup>Research Institute of Molecular Pathology (IMP), Vienna, Austria; <sup>2</sup>Institute of Molecular Biotechnology (IMBA), Vienna, Austria; <sup>3</sup>Gregor Mendel Institute of Molecular Plant Biology (GMI), Vienna, Austria
- MP 765 **Single-cell multi-omics analysis with Fucci3.2 cell cycle visualization probes;** Yoshihiro Izumi<sup>1</sup>; Kosuke Hata<sup>1</sup>; Asako Sawano<sup>2</sup>; Masatomo Takahashi<sup>1</sup>; Mamoru Hirafuji<sup>3</sup>; Kohta Nakatani<sup>1</sup>; Masaki Matsumoto<sup>4</sup>; Atsushi Miyawaki<sup>2, 5</sup>; Takeshi Bamba<sup>1</sup>; <sup>1</sup>Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; <sup>2</sup>RIKEN Center for Brain Science, Waco, Japan; <sup>3</sup>YODAKA Co., Ltd., Kawasaki, Japan; <sup>4</sup>Graduate School of Medical and Dental Sciences, Niigata University, Niigata, Japan; <sup>5</sup>RIKEN Center for Advanced Photonics, Wako, Japan
- MP 766 **Robust workflow for high-throughput quantitative analysis of low samples amounts and single-cells;** Tabiwang N. Arrey<sup>1</sup>; Santosh Renuse<sup>2</sup>; Jenny Ho<sup>3</sup>; Min Huang<sup>4</sup>; Shio Watanabe<sup>5</sup>; David Hartlmayr<sup>6</sup>; Anjali Seth<sup>6</sup>; Bernard Delanghe<sup>7</sup>; Nicolaie Eugen Damoc<sup>7</sup>; <sup>1</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>2</sup>ThermoFisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; <sup>4</sup>Thermo Fisher Scientific, Shanghai, China; <sup>5</sup>Thermo Fisher Scientific, Yokohama, Japan; <sup>6</sup>Cellenion, Lyon, France; <sup>7</sup>Thermo Fisher Scientific, Bremen, Germany
- MP 767 **Ultra-high throughput workflow for robust and sensitive quantitative single cell analysis;** Bernard Delanghe<sup>1</sup>; Julia Kraegenbring<sup>2</sup>; Tabiwang Arrey<sup>2</sup>; Fernanda Salvato<sup>3</sup>; David Hartlmayr<sup>4</sup>; Anjali Seth<sup>4</sup>; Eugen Damoc<sup>2</sup>; Tonya Pekar Hart<sup>3</sup>; Thomas Moehring<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; <sup>3</sup>ThermoFisher Scientific, San Jose, CA; <sup>4</sup>Cellenion, Lyon, France
- MP 768 **Exploring the Influence of the Number of Ions on Peptide Fragmentation Spectra;** Teeradon Phlairaham<sup>1</sup>; Brian Searle<sup>2</sup>; <sup>1</sup>Technical University of Munich (TUM), Freising, Germany; <sup>2</sup>Ohio State University, Columbus, OH
- MP 769 **Towards Preparation of 10k Single Cells Per Day for Tandem Mass Tag-based Single-cell Proteomics;** Ximena Sanchez-Avila<sup>1</sup>; H. Lavender Lin<sup>1</sup>; Tyler Hunter<sup>1</sup>; Kei

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- MP 770 **Enabling scalable single-cell proteomics by utilizing the unique analytical properties of the Evotip Pure**; Frederik Haugaard Vrdlovec Holck<sup>1</sup>; David Hartmayr<sup>2</sup>; Anjali Seth<sup>2</sup>; Ole Hoerning<sup>1</sup>; Dorte B. Bekker-Jensen<sup>1</sup>; Nicolai Bache<sup>1</sup>; <sup>1</sup>Evosep, Odense, Denmark; <sup>2</sup>Cellenion, Lyon, France
- MP 771 **Single-cell proteomic analysis of prostate cancer cell lines using a proteoCHIP-based TMT method**; Shimin Chen<sup>1</sup>; Vanessa Correll<sup>1</sup>; O. John Semmes<sup>1</sup>; Julius O. Nyalwidhe<sup>1</sup>; <sup>1</sup>Eastern Virginia Medical School, Norfolk, VA
- MP 772 **Multicolumn low-flow nanoLC-MS platform for high-throughput label-free single-cell proteomics**; Chao Wang<sup>1</sup>; Siqi Huang<sup>1</sup>; Kei Webber<sup>1</sup>; Thy Truong<sup>1,2</sup>; Xiaofeng Xie<sup>1,2</sup>; Ryan T. Kelly<sup>1</sup>; <sup>1</sup>Brigham Young University, Provo; <sup>2</sup>MicrOmics Technologies, Spanish Fork, UT
- MP 773 **Dissecting mammary stem cell heterogeneity in high-risk breast with a droplet-based low-input proteomic platform**; Matthew Waas<sup>1,2</sup>; Amanda Khoo<sup>1,2</sup>; Pirashaanthy Tharmapalan<sup>1</sup>; Curtis W McCloskey<sup>1</sup>; Meinusha Govindarajan<sup>1,2</sup>; Bowen Zhang<sup>1,2</sup>; Shahbaz Khan<sup>1</sup>; Paul Waterhouse<sup>1</sup>; Rama Khokha<sup>1,2</sup>; Thomas Kislinger<sup>1,2</sup>; <sup>1</sup>Princess Margaret Cancer Centre, University Health Network, Toronto, ON; <sup>2</sup>University of Toronto, Toronto, ON
- MP 774 **Deciphering Spatial Variation in Lipid Profiles of X-Ray Irradiated Cells using nLC and Orbitrap 240 MS**; Rahul Ravi Deshpande<sup>1</sup>; Kyle D.G. Saunders<sup>2</sup>; Johanna Gerichten<sup>2</sup>; Bashar Amer<sup>1</sup>; Thomas Moehring<sup>3</sup>; Melanie Bailey<sup>2</sup>; Susan S Bird<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Department of Chemistry, University of Surrey, Guildford, United Kingdom; <sup>3</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- MP 775 **Combining multiplexing with triggered MS/MS acquisition using super heavy TMT for targeted single cell proteomics**; Firdous A. Bhat<sup>1</sup>; Dong-Gi Mun<sup>1</sup>; Anu Jain<sup>1</sup>; Hiroshi Nishida<sup>1</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, MN 55905, USA
- MP 776 **Untargeted single cell lipidomics using ion mobility spectrometry**; Seul Kee Byeon<sup>1</sup>; Jinyong Kim<sup>1</sup>; Dong-Gi Mun<sup>1</sup>; Erica Marie Forsberg<sup>2</sup>; Sven W Meyer<sup>3</sup>; Aiko Barsch<sup>3</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN; <sup>2</sup>Bruker Scientific, Billerica, MA; <sup>3</sup>Bruker Daltonics GmbH & Co. KG, Billerica, MA
- MP 777 **Towards spatially-resolved proteome mapping at single-cell resolution with laser ablation**; Liang Chen<sup>1</sup>; Yumi Kwon<sup>1</sup>; Andrey V. Liyu<sup>1</sup>; Julia Unsworth<sup>2</sup>; Lye Meng Markillie<sup>1</sup>; Dehong Hu<sup>1</sup>; Rashmi Kumar<sup>1</sup>; Sarah M. Williams<sup>1</sup>; Megan K. Ruhland<sup>2</sup>; Ying Zhu<sup>3</sup>; Ljiljana Paša-Tolić<sup>1</sup>; <sup>1</sup>Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99352, USA., Richland, WA; <sup>2</sup>Department of Cell, Developmental and Cancer Biology, Knight Cancer Institute, Oregon Health and Science University, Portland, Oregon; <sup>3</sup>Department of Microchemistry, Proteomics, Lipidomics and Next Generation Sequencing, Genentech, South San Francisco, CA
- MP 778 **Thermal Inkjetting Enabled Single-Cell Proteomics for Evaluating Outcomes of Genetic Manipulations and Tracking Bioengineered Proteins in Individual Cells**; Stanislau Stanisheuski<sup>1</sup>; Hyo Sang Jang<sup>2</sup>; Kavi Aashish Vaidya<sup>1</sup>; Alex Eddins<sup>1</sup>; Liping Yang<sup>1</sup>; Jeffrey Morre<sup>1</sup>; Claudia S. Maier<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR; <sup>2</sup>HP Inc, Corvallis, OR
- MP 779 **Deciphering Cellular Responses to Abiotic and Biotic Stress through Single-Cell Proteomics**; James M Fulcher<sup>1</sup>; Pranav Dawar<sup>1</sup>; Vimal Balasubramanian<sup>2</sup>; Tanya Winkler<sup>2</sup>; Sarah M Williams<sup>2</sup>; Amir Ahkami<sup>2</sup>; Ljiljana Paša-Tolić<sup>2</sup>; Ying Zhu<sup>3</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>3</sup>Genentech Inc, South San Francisco, CA
- MP 780 **The Proteomics Landscape of PC12 Cells: Insights into Molecular Processes During Neuronal Differentiation and Maturation**; Arpa Ebrahimi<sup>1</sup>; Shuxin Chi<sup>2</sup>; Phoebe Lee<sup>3</sup>; Prongbamee Colling<sup>3</sup>; Liping Yang<sup>3</sup>; Luke C Marney<sup>3</sup>; Leonard J Foster<sup>2</sup>; Claudia S. Maier<sup>3</sup>; <sup>1</sup>OSU, Corvallis, OR; <sup>2</sup>University of British Columbia, Vancouver, BC; <sup>3</sup>Oregon State University, Corvallis

SMALL MOLECULES: QUALITATIVE AND QUANTITATIVE ANALYSIS  
781-803

- MP 781 **Standardizing retention times to reduce ambiguity of small molecule identification**; Huaxu Yu<sup>1</sup>; Tong Shen<sup>1</sup>; Jeremiah Wells<sup>1</sup>; Gert Wohlgemuth<sup>1</sup>; Uri Keshet<sup>1</sup>; Yendry Carvajal Miranda<sup>1</sup>; Yuanyue Li<sup>1</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>West Coast Metabolomics Center, University of California, Davis, Davis, CA
- MP 782 **Understanding small aromatic systems fragmentation pathways of historic anthraquinone dyes from the Max Weaver Dye Library**; Morgan Demmler<sup>1</sup>; Nelson Vinuesa<sup>1,2</sup>; <sup>1</sup>Wilson College of Textiles, NC State University, Raleigh, NC; <sup>2</sup>Department of Chemistry, NC State University, Raleigh, NC
- MP 783 **Optimization of AGC target value to improve quantitation accuracy of trace-level analyte by orbitrap mass spectrometer**; Eric M Brown<sup>1</sup>; Jingyue Yang<sup>1</sup>; Tim Marzan<sup>1</sup>; Dan Berger<sup>2</sup>; Ee-Sunn Chia<sup>2</sup>; Obinna Ugwu-Oju<sup>2</sup>; Mohammad Mohiminul Islam<sup>2</sup>; Rachel Dunn<sup>1</sup>; Alicia Hoover<sup>1</sup>; <sup>1</sup>Food and Drug Administration, St. Louis, MO; <sup>2</sup>Food and Drug Administration, Silver Spring, MD
- MP 784 **Impact of Mobile Phase Additive on APCI- and ESI-MS Ionization and In-Source Fragmentation of N-Nitrosamine Compounds**; Jessica N. Hoskins<sup>1</sup>; Monika Ladavicius<sup>2</sup>; John T. Lawler<sup>1</sup>; Richard A. Blessing<sup>1</sup>; Russell L. Hertzler<sup>1</sup>; <sup>1</sup>AbbVie, North Chicago, IL; <sup>2</sup>University of Minnesota, Minneapolis, MN
- MP 785 **Development of an assay for atropine in rabbit plasma by LC/MS/MS and the impact of atropine esterase**; Jean-François Larocque<sup>1</sup>; Jeff Plomley<sup>1</sup>; Anahita Keyhani<sup>1</sup>; <sup>1</sup>Altasciences, Laval, QC
- MP 786 **An LC-MS/MS method for bioanalysis of a molecular glue, pomalidomide, at sub-ng/mL levels in human plasma**; Eshani Galermo<sup>1</sup>; Ebru Selen<sup>1</sup>; Rahul Baghla<sup>1</sup>; <sup>1</sup>SCIEX, Redwood City, CA
- MP 787 **RECENT AUSTRALIAN FLAVOUR RESTRICTIONS: ANALYSING THE CHEMICAL PROFILES OF "TOBACCO" AND "MINT" ELECTRONIC CIGARETTES**; Caitlin Jenkins<sup>1,2</sup>; Jody Morgan<sup>1,2</sup>; Celine Kelso<sup>1,2</sup>; <sup>1</sup>School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; <sup>2</sup>Molecular Horizons, University of Wollongong, Wollongong, Australia
- MP 788 **Chip-Based CE-MS Analysis of Serotonin in the Rodent Fetus During Early Brain Development – the Placental Brain-Axis**; Chen Huang<sup>1</sup>; Jessica Kincade<sup>2</sup>; Cheryl S. Rosenfeld<sup>2</sup>; R. Michael Roberts<sup>2</sup>; Jonathan Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign, Urbana, IL; <sup>2</sup>University of Missouri-Columbia, Columbia, MO
- MP 789 **A Sensitive and Robust Assay for Simultaneous Quantification of Methylprednisolone Acetate and Methylprednisolone in Human Plasma Treated with Sodium Fluoride**; Molly McBride<sup>1</sup>; Charlie Zha<sup>2</sup>; Natasha Morgan<sup>1</sup>; Aihua Liu<sup>1</sup>; <sup>1</sup>Resolian (Formerly Alliance Pharma), Malvern, PA; <sup>2</sup>Brii Biosciences, Durham, NC
- MP 790 **An Ultra-Sensitive, High-Throughput, and Robust Assay to Quantify two Drug Conjugate Payloads (CRCPAC90045 and CRCPAC90978) in Human Plasma Using HPLC-MS/MS**; Hongfang (Andy) Xue<sup>1</sup>; Robert Huang<sup>2</sup>; Limin Chu<sup>1</sup>; Mo Xu<sup>2</sup>; Min Meng<sup>1</sup>; Gu tao Wang<sup>2</sup>; Yuehui Ma<sup>1</sup>; Fan Pan<sup>2</sup>; Aining Li<sup>2</sup>; Aihua Liu<sup>1</sup>; <sup>1</sup>Resolian (Formerly Alliance Pharma), Malvern, PA; <sup>2</sup>Coherent Biopharma, Hefei, China
- MP 791 **Enantiomer differentiation using magnesium adduct complexes and tandem mass spectrometry: towards**

## MONDAY POSTERS

- chiral recognition in metabolomics analyses;** Chenqin Cao<sup>1</sup>; Sandra Alves<sup>2</sup>; Jean-Claude Tabet<sup>1, 2</sup>; François Fenaillé<sup>1</sup>; Christophe Junot<sup>1</sup>; Annelaure DAMONT<sup>1</sup>; <sup>1</sup>Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), MetaboHUB, Gif-sur-yvette, France; <sup>2</sup>Faculté des Sciences et de l'Ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Sorbonne Université, Paris, France
- MP 792 **A Novel Assay to Measure Intracellular Endogenous Nucleotides and Active Antiretroviral Nucleotide Metabolites in Cell Lysate by LC-MS/MS;** Amanda P Schauer<sup>1</sup>; Craig Sykes<sup>1</sup>; Mackenzie L Cottrell<sup>1</sup>; Angela DM Kashuba<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC
- MP 793 **Markers of Degradation: Exploring the Oxidation of Polysorbate 80 and Polysorbate 20 with Ultra-High-Performance Liquid Chromatography and High-Resolution Mass Spectrometry;** Janez Mravljak<sup>1</sup>; Stane Pajk<sup>1</sup>; Ema Valentina Brovč<sup>2</sup>; Tinkara Lekić<sup>2</sup>; <sup>1</sup>University of Ljubljana, Faculty of Pharmacy, Ljubljana, Slovenia; <sup>2</sup>Novartis Pharmaceutical Manufacturing LLC, Menges, Slovenia
- MP 794 **Determination of Nitrosamine Impurities and NDSRI in Anti-diabetic Drugs on Shimadzu LCMS-8060NX;** Shao Hua Chia<sup>1</sup>; Siew Qi Yap<sup>1</sup>; Zhi Wei Edwin Ting<sup>1</sup>; <sup>1</sup>Shimadzu (Asia Pacific), Singapore, Singapore
- MP 795 **LC-MS Method for the Detection and Quantitation of Fermentation End-Products in Spent Media;** Erin R. Tiede<sup>1</sup>; Dam Soh<sup>2</sup>; Patricia I. Diaz<sup>2</sup>; Valerie Frerichs<sup>1</sup>; <sup>1</sup>Chemistry Instrument Center, Department of Chemistry, University at Buffalo, State University of New York, Buffalo, NY; <sup>2</sup>Department of Oral Biology, School of Dental Medicine, University at Buffalo, State University of New York, Buffalo, NY
- MP 796 **LC-QTOF Profiling of N-acyl-Homoserine Lactones Produced by Chromobacterium spp.;** Luer Wang<sup>1</sup>; Remy Kargodorian<sup>1</sup>; Alisha Harrison<sup>2</sup>; Scott Soby<sup>2</sup>; Charles A. Veltri<sup>3</sup>; <sup>1</sup>Midwestern University College of Dental Medicine, Glendale, Arizona; <sup>2</sup>Midwestern University College of Biomedical Sciences, Glendale, Arizona; <sup>3</sup>Midwestern University College of Pharmacy-Glendale, Glendale, AZ
- MP 797 **Comparison of Exhaled Breath Condensate Markers Using Two Ionization Methods: Electrospray Ionization and Dielectric Barrier Discharge Ionization;** Tatiana Rodriguez<sup>1</sup>; Lia Ficaró<sup>2</sup>; Drew R Jones<sup>2</sup>; Rebecca Jones<sup>2</sup>; <sup>1</sup>NYU Langone, Long Island City, NY; <sup>2</sup>NYU Langone, New York, NY
- MP 798 **Bioanalysis of lipid nanoparticle compounds in mouse and monkey plasma using LC-MS/MS;** Changyu Quang<sup>1</sup>; Joelle Lucarelli<sup>1</sup>; Brad Bessette<sup>1</sup>; Samuel Brown<sup>1</sup>; Morgan Trimmer<sup>1</sup>; Maryam Goudarzi<sup>1</sup>; Liam Moran<sup>1</sup>; Dhananjaya Nayak<sup>2</sup>; Sushimit Maitra<sup>3</sup>; <sup>1</sup>Charles River, Ashland, OH; <sup>2</sup>Charles River Laboratories, Worcester, MA; <sup>3</sup>Orna Therapeutics, Watertown, Massachusetts
- MP 799 **Enhancing Short-Chain Fatty Acids Quantification via GC-MS: Precipitation of Bromine Ions;** Cristina Arciniega<sup>1</sup>; Brandie M. Ehrmann<sup>1</sup>; <sup>1</sup>The University of North Carolina at Chapel Hill, Chapel Hill, NC
- MP 800 **Fragmentation and Ionization Behavior of Synthetic, Anthraquinone Disperse Dyes;** Zoe J Millbern<sup>1</sup>; Nelson R Vinuesa<sup>1</sup>; <sup>1</sup>NC State University, Raleigh, NC
- MP 801 **Overcoming Challenges: Bioanalytical Support for Incurred Sample Reanalysis Failure during LC-MS/MS Analysis of Human Plasma Samples in Phase I Study;** Komal Kothari<sup>1</sup>; Ryan Johnson<sup>1</sup>; Xiaorong Liang<sup>1</sup>; Brian Dean<sup>1</sup>; Michael Van Parys<sup>2</sup>; <sup>1</sup>Genentech Inc, South San Francisco, CA; <sup>2</sup>Labcorp Bioanalytical Services LLC, Indianapolis, IN
- MP 802 **Fast Isocratic LC/MS Orbitrap Method for the Simultaneous Quantitation of Uridine and Pseudouridine in Biological Samples;** Pradnya Patil<sup>1</sup>; Ling Fu<sup>2</sup>; Daniel Röth<sup>1</sup>; Yingfeng Deng<sup>2</sup>; Markus Kalkum<sup>1</sup>; <sup>1</sup>City of Hope, Beckman Research Institute, Department of Immunology and Theranostics, Duarte, CA; <sup>2</sup>City of Hope, Beckman Research Institute, Department of Diabetes and Cancer Metabolism, Duarte, CA
- MP 803 **Highly Sensitive and Selective Method for Estimation of Formoterol at Sub-pg/mL in Human Plasma Using Shimadzu LCMS-8060NX;** Avinash B Gaikwad<sup>1</sup>; Chaitanya Krishna Atmakuri<sup>1</sup>; Yogesh G Arote<sup>1</sup>; <sup>1</sup>ADC-Shimadzu Analytical India Pvt Ltd, NAVI MUMBAI, India

### VIRUSES AND VIRUS-LIKE PARTICLES 804-821

- MP 804 **LC-MS based Peptide Mapping Methods for Characterization of Gene Therapy Vector Proteins;** Yu Zhou<sup>1</sup>; Derek Langeslay; <sup>1</sup>Novartis, San Diego, CA
- MP 805 **Detection and relative quantitation of host cell proteins in lentivirus preparations;** Sahana Mollah<sup>1</sup>; Remco Van Soest<sup>1</sup>; Alicia Powers<sup>2</sup>; Chao-Xuan Zhang<sup>2</sup>; Timothy Lockey<sup>2</sup>; <sup>1</sup>SCIEX, Redwood City, CA; <sup>2</sup>St.Jude Children's Research Hospital, Memphis, TN
- MP 806 **Recombinant Extracellular Vesicles as Tools for Membrane Protein Interactomics;** Shengya Cao<sup>1</sup>; Sean M Peterson<sup>1</sup>; Soren Muller<sup>1</sup>; Mike Reichelt<sup>1</sup>; Christian McRoberts Amador<sup>2</sup>; Nadia Martinez-Martin<sup>1</sup>; <sup>1</sup>Genentech Inc, South San Francisco, CA; <sup>2</sup>Duke University, Durham, NC
- MP 807 **Comparison of the Empty/Full ratio assessment by Direct Mass Technology, Analytical Ultracentrifugation and Mass Photometry for AAV vectors;** Ryoji Nakatsuka<sup>1, 2, 3</sup>; Yuki Yamaguchi<sup>1</sup>; Tatsuya Aisu<sup>1</sup>; Kiichi Hiroyhata<sup>1</sup>; Saki Shimojo<sup>1</sup>; Aoba Matsushita<sup>1</sup>; Yasuo Tsunaka<sup>1</sup>; Mitsuko Fukuhara<sup>1, 4</sup>; Tetsuo Torisu<sup>1</sup>; Susumu Uchiyama<sup>1</sup>; <sup>1</sup>Osaka university, Osaka, Japan; <sup>2</sup>Shimadzu Corporation, Nakagoyoku, Japan; <sup>3</sup>Osaka University Shimadzu Analytical Innovation Research Laboratories, Suita-shi, Japan; <sup>4</sup>U-Medico Inc, Suita-shi, Japan
- MP 808 **Tracking host cell protein (HCP) clearance on adeno-associated virus (AAV) products generated using HEK and Sf9 production systems;** Josh Smith<sup>1</sup>; Aaron Richardson<sup>1</sup>; Sara Carillo<sup>1</sup>; Marina Ainciburu<sup>1</sup>; Ioanna Tzani<sup>1</sup>; Michelle Chain<sup>1</sup>; Colin Clarke<sup>1, 2</sup>; Eugen Damoc<sup>3</sup>; Jonathan Bones<sup>1, 2</sup>; <sup>1</sup>The National Institute for Bioprocessing Research & Training, Dublin, Ireland; <sup>2</sup>School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland; <sup>3</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- MP 809 **A combination of lectin-based fractionation and LC-MS/MS for glycosylation analysis of recombinant adeno-associated virus;** Yuki Yamaguchi<sup>1</sup>; Kentaro Ishii<sup>1</sup>; Sachiko Koizumi<sup>2, 3</sup>; Hiroaki Sakaue<sup>4</sup>; Takahiro Maruno<sup>1, 5</sup>; Mitsuko Fukuhara<sup>1, 5</sup>; Risa Shibuya<sup>1</sup>; Yasuo Tsunaka<sup>1</sup>; Aoba Matsushita<sup>1</sup>; Karin Bandoh<sup>1</sup>; Tetsuo Torisu<sup>1</sup>; Chie Murata-Kishimoto<sup>2</sup>; Azusa Tomioka<sup>4</sup>; Saho Mizukado<sup>4</sup>; Hiroyuki Kaji<sup>6</sup>; Yuji Kashiwakura<sup>7</sup>; Tsukasa Ohmori<sup>7</sup>; Atsushi Kuno<sup>4</sup>; Susumu Uchiyama<sup>1</sup>; <sup>1</sup>Osaka University, Suita, Japan; <sup>2</sup>GlycoTechnica Ltd., Yokohama, Japan; <sup>3</sup>Precision System Science Co. Ltd., Matsudo, Japan; <sup>4</sup>National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; <sup>5</sup>U-Medico Inc., Suita, Japan; <sup>6</sup>Nagoya University, Nagoya, Japan; <sup>7</sup>Jichi Medical University, Shimotsuke, Japan
- MP 810 **Key Applications of ELIT CDMS;** Rebecca J. D'Esposito<sup>1</sup>; Anisha Haris<sup>2</sup>; David Bruton<sup>2</sup>; Kevin Giles<sup>2</sup>; Keith G Richardson<sup>2</sup>; Chris Wheelodon<sup>2</sup>; Alistair Schofield<sup>2</sup>; David Eatough<sup>2</sup>; Ying Qing Yu<sup>1</sup>; Steve Preece<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom
- MP 811 **Optimizing Mass Spectrometer Conditions to Accurately Determine Full/Empty AAV Ratios: A Sample Half-Full Approach;** Kyle Patrick Bowen<sup>1</sup>; Michael Goodwin<sup>1</sup>; Michael W Senko<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA
- MP 812 **Characterization of Adeno-Associated Virus (AAV9) Capsid Proteoforms using Multiple Ion Activations on an Orbitrap Tribrid Instrument;** Rafael D Donadelli Melani<sup>1</sup>;

## MONDAY POSTERS

- Kristina Srzentic<sup>2</sup>; Jingjing Huang<sup>1</sup>; Jake T Kline<sup>3</sup>; Christopher Mullen<sup>1</sup>; Luca Fornelli<sup>3</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Reinach, Switzerland*; <sup>3</sup>*University of Oklahoma, Norman, OK*
- MP 813 **Characterisation of Adeno Associated Virus Capsid Proteins using Top-Down LC-MS/MS**; Felipe Guapo<sup>1</sup>; Corentin Beaumal<sup>1</sup>; Josh Smith<sup>1</sup>; Silvia Millan Martin<sup>1</sup>; Sara Carillo<sup>1</sup>; Jonathan Bones<sup>1, 2</sup>; <sup>1</sup>*The National Institute for Bioprocessing Research & Training, Dublin, Ireland*; <sup>2</sup>*School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland*
- MP 814 **Mass Spectrometry based characterization and identification of an N-terminal acetylated viral capsid protein 2 in Adeno-associated virus capsid proteins**; Ruiyi Dong<sup>1</sup>; Dingyi Wen<sup>1</sup>; Malgorzata Szyjka<sup>1</sup>; Xiaofeng Yang<sup>1</sup>; Paul Weinreb<sup>1</sup>; <sup>1</sup>*Biogen, Biologicals Drug Discovery, Cambridge, MA*
- MP 815 **Optimization of Adeno-Associated Virus peptide mapping using trapped ion mobility spectrometry**; Isin T Sakallioğlu<sup>1</sup>; Anjali Alving<sup>1</sup>; Guillaume Tremintin<sup>2</sup>; <sup>1</sup>*Bruker Scientific, LLC, Billerica, MA*; <sup>2</sup>*Bruker Scientific LLC, San Jose, CA*
- MP 816 **Automated Quantitation of Adeno-Associated Virus Byproducts Using Individual Ion Mass Spectrometry**; Ryan T. Fellers<sup>1, 2</sup>; Michael A. R. Hollas<sup>1</sup>; Bryan P. Early<sup>1</sup>; Joseph B. Greer<sup>1, 2</sup>; Kenneth R. Durbin<sup>2</sup>; Mike Goodwin<sup>3</sup>; Ping Yip<sup>3</sup>; Kristina Srzentic<sup>3</sup>; Kyle P. Bowen<sup>3</sup>; Michael W. Senko<sup>3</sup>; Samuel E. Janisse<sup>1</sup>; Jared Kafader<sup>1</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>*Northwestern University, Evanston, IL*; <sup>2</sup>*Proteinaceous, Inc., Evanston, IL*; <sup>3</sup>*Thermo Fisher Scientific – 355 River Oaks Pkwy, San Jose, California*
- MP 817 **Profiling HIV-1 Virion Complexity at the Proteoform Level**; Claire E. Boos<sup>1</sup>; Mark Scalf<sup>1</sup>; James W. Bruce<sup>2, 3</sup>; Rachel M. Miller<sup>1</sup>; Nathan M. Sherer<sup>2, 3</sup>; Lloyd M. Smith<sup>1</sup>; <sup>1</sup>*University of Wisconsin-Madison, Department of Chemistry, Madison, WI*; <sup>2</sup>*McArdle Laboratory for Cancer Research, University of Wisconsin-Madison, Madison, WI*; <sup>3</sup>*Institute for Molecular Virology, Madison, WI*
- MP 818 **The metabolic basis of dengue virus NS1-induced vascular leak in mouse tissues**; Paul S. Soma<sup>1</sup>; Jaime Cardona-Ospina<sup>2</sup>; Barbara Graham<sup>1</sup>; Hannah Laurence<sup>1</sup>; Scott B. Biering<sup>2</sup>; Eva Harris<sup>2</sup>; Rushika Perera<sup>1</sup>; <sup>1</sup>*Department of Microbiology, Immunology and Pathology, Center for Metabolism of Infectious Diseases, Colorado State University, Fort Collins, Colorado*; <sup>2</sup>*Division of Infectious Diseases and Vaccinology, School of Public Health, University of California, Berkeley, Berkeley, California*
- MP 819 **Huge and Heterogeneous: Probing Biophysical Properties of Lipid Nanoparticles and Viruses with Charge Detection Mass Spectrometry**; Zachary M. Miller<sup>1</sup>; Li F. Lin<sup>1</sup>; David V. Schaffer<sup>1</sup>; Justin W. Torpey<sup>2</sup>; Lokesh Narsineni<sup>2</sup>; Yue-xuan Li<sup>2</sup>; Matthew R. Gardner<sup>2</sup>; Evan R. Williams<sup>1</sup>; <sup>1</sup>*University of California, Berkeley, Berkeley, CA*; <sup>2</sup>*Scribe Therapeutics, Alameda, CA*
- MP 820 **Characterization of Bacteriophage P22 Procapsid and Wiffle Ball Structures by Charge Detection Mass Spectrometry**; Luke W. Hawkins<sup>1</sup>; Isaiah R. Moss<sup>1</sup>; Shelby M. Klein<sup>1</sup>; Martin F. Jarrold<sup>1</sup>; <sup>1</sup>*Indiana University Bloomington, Bloomington, IN*
- MP 821 **Enabling icIEF Peak Identification: AAV Capsid Protein Fractionation on MauriceFlex and Subsequent Analysis by LC-MS**; Xiaoping He<sup>1</sup>; Sisi Huang<sup>1</sup>; Will McElroy<sup>2</sup>; Melissa Anderson<sup>1</sup>; Courtney Sloan<sup>1</sup>; Thomas Powers<sup>1</sup>; Chris Heger<sup>2</sup>; Tom Lerch<sup>1</sup>; <sup>1</sup>*Pfizer Inc, Chesterfield, MO*; <sup>2</sup>*ProteinSimple, Bio-Techne, San Jose, CA*

## TUESDAY POSTERS

### TUESDAY POSTERS

Set up all Tuesday posters  
6:30 - 9:00 am

**Odd-numbered posters present**  
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

**Even-numbered posters present**  
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Tuesday posters  
5:00 - 8:00 pm

Ambient Ionization: Applications II.....	001-021
Biomarkers: Quantitative Analysis I.....	022-047
Disease Biomarkers.....	048-062
Environmental: General II.....	063-098
Exposomics.....	099-117
Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements II.....	118-137
Fundamentals: Ion Molecule, Ion/Ion, Ion/Electron Interactions.....	138-154
Fundamentals: Native MS.....	155-171
High Throughput MS I.....	172-196
Imaging MS: Instrumentation.....	197-206
Imaging MS: Pharmaceuticals, Metabolites, Lipids, and Glycans II.....	207-229
Imaging: Spatially-Resolved Omics II.....	230-248
Informatics: Algorithms and Statistical Advances.....	249-283
Instrumentation: General.....	284-299
Ion Mobility: Applications II.....	300-319
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### AMBIENT IONIZATION: APPLICATIONS II 001-021

- TP 001 **Origins of Reaction Acceleration and Unusual Reactions in Charged Droplets**; Casey J. Chen<sup>1</sup>; Evan R. Williams<sup>1</sup>; <sup>1</sup>University of California, Berkeley, Berkeley
- TP 002 **A single prediction model for two ambient ionization mass spectrometry techniques: Applications in breast surgical margin assessment**; Laura Min Xuan Chai<sup>1</sup>; Ching Kao<sup>2</sup>; Ming-Yang Wang<sup>3</sup>; Cheng-Chih Hsu<sup>1, 4</sup>; <sup>1</sup>Department of Chemistry, National Taiwan University, Taipei, Taiwan; <sup>2</sup>Department of Medical Oncology, National Taiwan University Cancer Center, Taipei, Taiwan; <sup>3</sup>Department of Surgical Oncology, National Taiwan University Cancer Center, Taipei, Taiwan; <sup>4</sup>Leeuwenhoek Laboratories, Co. Ltd., Taipei, Taiwan
- TP 003 **Direct Dual Polarity Mass Spectrometry Imaging (DDPMSI) of Renal Cell Carcinoma**; Rachel Wood<sup>1</sup>; Malek Hassan<sup>1</sup>; Rachel L. Theriault<sup>2</sup>; Randy E. Ellis<sup>2, 3</sup>; Kevin Ren<sup>4</sup>; Richard D. Oleschuk<sup>1</sup>; <sup>1</sup>Department of Chemistry, Queen's University, Kingston, ON; <sup>2</sup>School of Computing, Queen's University, Kingston, ON; <sup>3</sup>Department of Surgery, Queen's University, Kingston, ON; <sup>4</sup>Department of Pathology and Molecular Medicine, Queen's University, Kingston, ON
- TP 004 **High Throughput DESI Tissue Analysis of Angiotensin II Metabolism in Mice**; Kenneth L. Virgin<sup>1, 2</sup>; Nicolás M. Morato<sup>2</sup>; R. Graham Cooks<sup>2</sup>; <sup>1</sup>Indiana University Indianapolis, Indianapolis, IN; <sup>2</sup>Purdue University, West Lafayette, IN
- TP 005 **Development of rapid screening methods for herbs used in Traditional Chinese Medicine (TCM)**; TIANHUI YU<sup>1</sup>; James Reynolds<sup>1</sup>; <sup>1</sup>Loughborough University, Loughborough, United Kingdom
- TP 006 **Automated Laser Assisted-Rapid Evaporative Ionisation Mass Spectrometry (LA-REIMS) for cell line phenotype prediction in real-time**; Paul Abu-Rabie; GSK, Stevenage, Hertfordshire, United Kingdom
- TP 007 **Non-Invasive Monitoring of Caffeine and Its Metabolites via Human Skin with Ambient Ionization Tandem Mass Spectrometry**; Kyung Hwa Kee<sup>1, 2</sup>; Chi-Yang Lee<sup>2</sup>; Jia-Cheng Chen<sup>2</sup>; Rui-Ying Hong<sup>2</sup>; Chun-Hsiu Chiu<sup>2</sup>; Hye Hyun Yoo<sup>1</sup>; Jentaie Shiea<sup>2</sup>; <sup>1</sup>College of Pharmacy, Hanyang University, Ansan, South Korea; <sup>2</sup>Department of Chemistry, National Sun Yat-sen University, Kaohsiung, Taiwan
- TP 008 **Ambient Ionization Mass Spectrometry Provides Screening of Selective Androgen Receptor Modulators**; Alzbeta Nemeskalova<sup>1</sup>; Jitka Konvalinkova<sup>1</sup>; Jan Bucek<sup>2</sup>; Magdalena Vagnerova<sup>1</sup>; Vladimir Vrkoslav<sup>3</sup>; David Sykora<sup>1</sup>; Martin Kuchar<sup>1</sup>; Josef Cvacka<sup>3</sup>; Michael Volny<sup>1, 4</sup>; <sup>1</sup>University of Chemistry and Technology Prague, Prague 6 - Dejvice, Czech Republic; <sup>2</sup>Plasmion GmbH, Augsburg, Germany; <sup>3</sup>Institute of Organic Chemistry and Biochemistry of the CAS, Prague 6 - Dejvice, Czech Republic; <sup>4</sup>Institute of Microbiology CAS, Prague 4 - Krc, Czech Republic
- TP 009 **Discovery and spatial mapping of novel truncated pancreatic peptides using nano-DESI MSI**; Mushfeqa Iqbal<sup>1</sup>; Manxi Yang<sup>1</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- TP 010 **A Platform for Scalable Green Carbon Dioxide and Nitrogen Fixation from Ambient Air Using Aqueous Microdroplets**; Dylan T. Holden<sup>1</sup>; Myles Q. Edwards<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University Department of Chemistry, West Lafayette, IN
- TP 011 **Application of rapid evaporative ionization mass spectrometry (REIMS) for the prediction of beef tenderness**; Sebastian Hernandez<sup>1</sup>; Kaitlyn Loomas<sup>1</sup>; Yifei Wang<sup>2</sup>; Dale Woerner<sup>1</sup>; Benjamin Bohrer<sup>2</sup>; Tyson Brown<sup>3</sup>; Heather Bruce<sup>4</sup>; Marcio Duarte<sup>5</sup>; Jerrad Legako<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, Texas; <sup>2</sup>The Ohio State University, Columbus, OH; <sup>3</sup>Cargill Meat Solutions, Wichita, Kansas; <sup>4</sup>University of Alberta, Edmonton, AB; <sup>5</sup>University of Guelph, Guelph, ON

## TUESDAY POSTERS

- TP 012 **Sheath-flow probe electrospray-mass spectrometry: A rapid ambient method for in-situ forensic analysis of fingerprints and biofluid residues.**; James C. Reynolds<sup>1</sup>; Ayoung Kim<sup>1</sup>; Matthew A. Turner<sup>1</sup>; Paul F. Kelly<sup>1</sup>; <sup>1</sup>Loughborough University, Loughborough, United Kingdom
- TP 013 **Online ultrafast trypsin digestion of LC-separated proteins using microdroplet digestion**; Praneeth Ivan Joel FNU<sup>1</sup>; Timothy Yaroshuk<sup>1</sup>; Mengyuan Xiao<sup>1</sup>; Md Tanim-Al Hassan<sup>1</sup>; Harsha Gunawardena<sup>2</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>New Jersey Institute of Technology, Newark, NJ; <sup>2</sup>JOHNSON AND JOHNSON, Spring House, PA
- TP 014 **Identification of Carpine in Carica papaya Leaf Products using Direct Analysis in Real Time Mass Spectrometry (DART-MS)**; Piyawadi Khaomiam<sup>1</sup>; Patanachai Limpikirati<sup>1, 2</sup>; Rossarin Tansawat<sup>1, 2</sup>; <sup>1</sup>Department of Food and Pharmaceutical Chemistry, Faculty of Pharmaceutical Sciences, Chulalongkorn University, Bangkok, Thailand; <sup>2</sup>Metabolomics for Life Sciences Research Unit, Chulalongkorn University, Bangkok, Thailand
- TP 015 **Direct and Indirect Thermal Desorption and Pyrolysis of Polymers by DART and GC-MS: A Hot Topic!**; Robert B Cody<sup>1</sup>; John Dane<sup>1</sup>; Kirk Jensen<sup>1</sup>; Bryan Katzenmeyer<sup>1</sup>; <sup>1</sup>JEOL USA, Inc., Peabody, MA
- TP 016 **Exploring the capability of the Waters™ RADIANT™ ASAP mass spectrometer for simple, rapid detection of antimicrobials in food and feed**; Annette O Farrell<sup>1</sup>; Panagiotis Manesiotis<sup>1</sup>; Simon Cameron<sup>1</sup>; <sup>1</sup>Queens University Belfast, Belfast, United Kingdom
- TP 017 **10-second Classification of Lung Cancer Subtypes by Picosecond Infrared Laser Mass Spectrometry: Evaluation of Diagnostic Power Across Various Tissue Models**; Lan Anna Ye<sup>1</sup>; Michael Woolman<sup>2</sup>; Francis Talbot<sup>1</sup>; Alexa Fiorante<sup>2</sup>; Yuki Sata<sup>3</sup>; Hiroyuki Ogawa<sup>3</sup>; Fumi Yokote<sup>3</sup>; Nicholas Bernards<sup>3</sup>; Michael Cabanero<sup>3</sup>; Nhu-An Pham<sup>1</sup>; Nikolina Radulovich<sup>1</sup>; Benjamin Lok<sup>1</sup>; Kazuhiro Yasufuku<sup>3</sup>; Ming-Sound Tsao<sup>1</sup>; Howard Ginsberg<sup>4</sup>; Arash Zarrine-Afsar<sup>5</sup>; <sup>1</sup>Princess Margaret Cancer Centre, University Health Network, Toronto, ON; <sup>2</sup>Department of Medical Biophysics, University of Toronto, Toronto, ON; <sup>3</sup>University Health Network, Toronto, Ontario; <sup>4</sup>Unity Health Toronto, St Michael's Hospital, Toronto, Ontario; <sup>5</sup>University of Toronto, Toronto, ON
- TP 018 **DPiMS-MS (PESI) combined with vacuum differential mobility spectrometry for rapid clinical/forensic analysis**; Gordon C Kearney<sup>1</sup>; Patrick Knight<sup>1</sup>; Andrew Entwistle<sup>1</sup>; Franck SAINT-MARCOUX<sup>2</sup>; Pauline GRIFFEUILLE<sup>2</sup>; Souleiman EL BALKHI<sup>2</sup>; Ann-Christin Ann-Christin Niehoff<sup>3</sup>; Stephane Moreau<sup>3</sup>; <sup>1</sup>Shimadzu Research Laboratory (Europe) Ltd., Manchester, United Kingdom; <sup>2</sup>University Hospital of Limoges, Limoges, France; <sup>3</sup>Shimadzu Europa GmbH, Duisburg, Germany
- TP 019 **Advanced Paper Spray Ionization Mass Spectrometry: Targeted Polyamine Odor Molecules Analysis by Aldehyde-Functionalized Cellulose Filter Paper**; Egodage Udeesha Inoshi De Silva<sup>1</sup>; Jianchuan Wen<sup>1</sup>; Yuyu Sun<sup>1</sup>; Anyin Li<sup>2</sup>; Pengyuan Liu<sup>1</sup>; <sup>1</sup>University of Massachusetts, Lowell, MA; <sup>2</sup>University of New Hampshire, Durham, NH
- TP 020 **GC-SICRIT-MS for Rapid Chemical Analysis of Electronic Cigarette Liquid**; Xiaoping Wang<sup>1</sup>; Xiaokun Duan<sup>1</sup>; Charles C. Liu<sup>1</sup>; <sup>1</sup>ASPEC Technologies, Suzhou, China
- TP 021 **Rapid Quantitative Screening of 18 Synthetic Cannabinoids in Urine Using DART-MS Analysis**; Terry L Bates<sup>1</sup>; William Fatigante<sup>2</sup>; Alex Maggitti<sup>3</sup>; Francois Espourteille<sup>2</sup>; <sup>1</sup>Bruker Scientific, Billerica, MA; <sup>2</sup>Bruker Scientific, LLC, Billerica, MA; <sup>3</sup>DrugScan, Inc., Horsham, PA
- TP 022 **Proteomic multi-marker model for diagnosis of obsessive compulsive disorder by multiple reaction monitoring-mass spectrometry**; Yeongshin Kim<sup>1</sup>; Dongyoon Shin<sup>2</sup>; Junho Park<sup>2, 3</sup>; Chun Il Park<sup>4</sup>; Se Joo Kim<sup>5</sup>; Youngsoo Kim<sup>1, 2</sup>; <sup>1</sup>Department of Medical Science, School of Medicine, CHA University, Pangyo, South Korea; <sup>2</sup>Proteomics Research Team, CHA Institute of Future Medicine, Pangyo, South Korea; <sup>3</sup>Department of Pharmacology, School of Medicine, CHA University, Pangyo, South Korea; <sup>4</sup>Department of Psychiatry, CHA Bundang Medical Center, CHA University, Pangyo, South Korea; <sup>5</sup>Department of Psychiatry, Yonsei University College of Medicine, South Korea
- TP 023 **Bile proteomics for identifying biomarkers to differentiate hepatobiliary diseases**; Hyunesoo Kwon<sup>1</sup>; Young Eun Kim<sup>2, 3</sup>; Pham Ha Chau<sup>2, 4</sup>; Hoeil Chung<sup>5</sup>; Dukjin Kang<sup>2</sup>; Tae-Young Kim<sup>1</sup>; <sup>1</sup>School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea; <sup>2</sup>Korea Research Institute of Standards and Science, Daejeon, South Korea; <sup>3</sup>Gwangju Institute of Science and Technology, Gwangju, South Korea; <sup>4</sup>Chungnam National University, Daejeon, South Korea; <sup>5</sup>Hanyang University, Seoul, South Korea
- TP 024 **Target and Probe Tm Guided Method Development Strategy for Hybridization LC-MS/MS Quantification of siRNA**; Zifeng Song<sup>1</sup>; Angela Lu<sup>1</sup>; Long Yuan<sup>1</sup>; <sup>1</sup>Biogen, Cambridge, MA
- TP 025 **prM-PASEF HT: High sensitivity and throughput for absolute quantitation of plasma proteins**; Simonas Savickas<sup>1</sup>; Sebastian Mueller<sup>1</sup>; Véronique Laforte<sup>1</sup>; Tejas Gandhi<sup>1</sup>; Roland Bruderer<sup>1</sup>; Lukas Reiter<sup>1</sup>; <sup>1</sup>Biognosys AG, Schlieren, Switzerland
- TP 026 **Improving Measurement Traceability in Untargeted Metabolomics: A Key to Cross-Study Comparisons**; Andre Märtens<sup>1, 2</sup>; Karsten Hiller<sup>2</sup>; Gavin O'Connor<sup>1, 2</sup>; <sup>1</sup>Physikalisch-Technische Bundesanstalt, Braunschweig, Germany; <sup>2</sup>Department of Bioinformatics and Biochemistry - Braunschweig Integrated Centre of Systems Biology, Braunschweig, Germany
- TP 027 **Want to know your stress level with a single swab and a few seconds of analysis? It's possible using LDTD-MS/MS**; Mégane Moreau<sup>1</sup>; Jonathan Rochon<sup>1</sup>; Sarah Demers<sup>1</sup>; Serge Auger<sup>1</sup>; Jean Lacoursière<sup>1</sup>; Pierre Picard<sup>1</sup>; <sup>1</sup>Phytronix Technologies, Quebec, QC
- TP 028 **Quantitative estimation of urine proteins for biomarker discovery by Data-independent acquisition mass spectrometry (DIA-MS)**; Tadashi Yamamoto<sup>1</sup>; Keiko Yamamoto<sup>1</sup>; <sup>1</sup>Niigata University, Biofluid Biomarker Center (BBC), Environmental/Energy Science Center 5F, Niigata, Japan
- TP 029 **Label-free quantitative proteomics characterizes immunopathogenesis of Chikungunya virus infection in hepatocellular carcinoma cells**; Sutopa Dwivedi; Emergex USA, Doylestown, PA
- TP 030 **Evaluating the extent of HIV-1 infection of mammalian cells by immunoaffinity enrichment, LC-MRM-QQQ quantitation of GP120 protein in MoltIIb cells**; Bao-Jen Shyong<sup>1</sup>; Matthew T. Mazur<sup>2</sup>; Guoxin Wu<sup>3</sup>; Brian C. Magliaro<sup>3</sup>; Weixun Wang<sup>1</sup>; <sup>1</sup>PDMB, MRL, Merck & Co., Inc., West Point, PA; <sup>2</sup>PDMB, MRL, Merck & Co., Inc., West Point, PA; <sup>3</sup>Biology-Discovery, MRL, Merck & Co., Inc., West Point, PA
- TP 031 **A multiplexed quantitative analysis of naturally occurring single amino acid variants by targeted proteomics in non-depleted human plasma**; Panshak Dakup<sup>1</sup>; Tai-Tu Lin<sup>1</sup>; Soumyadeep Sarkar<sup>1</sup>; Adam C Swensen<sup>1</sup>; Athena M Schepmoes<sup>1</sup>; Thomas L. Fillmore<sup>1</sup>; James P Delany<sup>2</sup>; Bret H Goodpaster<sup>2</sup>; Tujin Shi<sup>1</sup>; Wei-Jun Qian<sup>1</sup>; Jon M. Jacobs<sup>1</sup>; A2CPS Consortium<sup>3</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>AdventHealth Research Institute, Orlando, FL; <sup>3</sup>NIH Commonfund, Bethesda, MD
- TP 032 **Quantitative Assay for Diacylglycerol Kinase Kappa with Mass Spectrometry and Parallel Reaction Monitoring**; Oktay CAKIL<sup>1</sup>; Anastasiia PETROVA<sup>1</sup>; Luc NEGRONI<sup>1</sup>

**BIOMARKERS: QUANTITATIVE ANALYSIS I**  
022-047

## TUESDAY POSTERS

- Hervé MOINE<sup>1</sup>; <sup>1</sup>Université de Strasbourg, CNRS, Inserm, IGBMC UMR 7104- UMR-S 1258, F-67400 Illkirch, France, ILLKIRCH, France
- TP 033 **A sensitive determination of bisphenol A and its 11 analogs and triclosan in urine by UPLC-MS/MS;** Eric Gaudreau<sup>1</sup>; Sébastien Gagné<sup>1</sup>; Patrick Bélanger<sup>1</sup>; Normand Fleury<sup>1</sup>; <sup>1</sup>Centre de Toxicologie du Québec (CTQ/INSPQ), Québec, QC
- TP 034 **Systematic Evaluation of Proteomic Responses Related to Multisystem Proteinopathy 1 using iPSC-derived Cerebral Organoids;** Feng Wang<sup>1</sup>; Shan Li<sup>1</sup>; Baiyi Quan<sup>2</sup>; Tsui-Fen Chou<sup>1, 2</sup>; <sup>1</sup>Division of Biology and Biological Engineering, California Institute of Technology, Pasadena, CA; <sup>2</sup>Proteome Exploration Laboratory, Beckman Institute, California Institute of Technology, Pasadena, CA
- TP 035 **Towards Comprehensive Plasma Proteomics: Optimizing PRM-PASEF for Disease Biomarker Discovery;** Raghothama Chaerkady<sup>1</sup>; Morgan Fair<sup>1</sup>; Liang Zhao<sup>1</sup>; Qing Wang<sup>1</sup>; <sup>1</sup>CompleteOmics, Halethorpe, MD
- TP 036 **Unveiling Real-time Changes: In Vivo Solid Phase Microextraction of Ultra-Trace Endogenous Psychedelics;** Min Liu<sup>1,2</sup>; Oliver Fiehn<sup>1,2</sup>; David E. Olson<sup>2,3,4,5</sup>; Cassandra Hatzipantelis<sup>2,3,4,5</sup>; Yara Ahmad Khatib<sup>3</sup>; <sup>1</sup>West Coast Metabolomics Center, University of California Davis, Davis, CA; <sup>2</sup>Institute for Psychedelics and Neurotherapeutics, University of California, Davis, Davis, California; <sup>3</sup>Department of Chemistry, University of California, Davis, Davis, California; <sup>4</sup>Department of Biochemistry and Molecular Medicine, School of Medicine, University of California, Davis, Sacramento, California; <sup>5</sup>Center for Neuroscience, University of California, Davis, Davis, California
- TP 037 **Development of On-line Solid Phase Extraction LC/MS/MS Method for Quantification of 30 Bile Acids in Feces;** Amanda Blake<sup>1</sup>; Gabrielle Sakel<sup>1</sup>; Madison Perez<sup>1</sup>; Jake Chaconas<sup>1</sup>; Jan Suchodolski<sup>1</sup>; <sup>1</sup>Gastrointestinal Lab, Texas A&M University, College Station, TX
- TP 038 **A High-Throughput, In-Depth Investigation into the Immunological Effects of Lipopolysaccharide Challenged Mice in Neat Plasma on Orbitrap Astral Mass Spectrometer;** Jana Richter<sup>1</sup>; Nicolas Hartel<sup>1</sup>; Kevin Yang<sup>1</sup>; Amirmansoor Hakimi<sup>1</sup>; Stephanie Samra<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA
- TP 039 **Optimization of mass spectrometry methods for longitudinal measurement of biomarkers in Duchenne muscular dystrophy;** Ahmed Naveed<sup>1</sup>; Yubin Ki<sup>1</sup>; Elissa Recinos<sup>1</sup>; Dexter Chow<sup>1</sup>; Emily Canessa<sup>1</sup>; Yetric Hathout<sup>1</sup>; <sup>1</sup>Binghamton University-SUNY, Binghamton, NY
- TP 040 **Multi-Omics for Plasma: A Three-in-One End-to-End Automated Sample Preparation and LC/MS Metabolomics, Lipidomics, and Proteomics Workflow;** Christian Klein<sup>1</sup>; Karen E Yannell<sup>1</sup>; Cate Simmermaker<sup>1</sup>; Sierra D. Durham<sup>1</sup>; Genevieve Van De Bittner<sup>1</sup>; Mark Sartain<sup>1</sup>; Sheher Banu Mohsin<sup>1</sup>; Linfeng Wu<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- TP 041 **Seasonal variation of neonicotinoids and their metabolites in Iowa surface and groundwaters;** Wenjing Xi; <sup>1</sup>Center for Health Effects of Environmental Contamination at the University of Iowa, Iowa City, Iowa
- TP 042 **Hydrophilic Interaction Liquid Chromatography Mass Spectrometry Enables Cellular Assay Development to Identify Inhibitors of Glycine N-Methyltransferase;** Jonathan Shrimp<sup>1</sup>; Quinlin Hanson<sup>1</sup>; Nate Hoxie<sup>1</sup>; John Janiszewski<sup>1</sup>; Vinoth Chenniappan<sup>1</sup>; Colin Kelly<sup>1</sup>; Min Shen<sup>1</sup>; Samarjit Patnaik<sup>1</sup>; Matthew D Hall<sup>1</sup>; <sup>1</sup>NCATS/NIH, Rockville, MD
- TP 043 **High-throughput Quantification of 802 Peptides in Blood Plasma using 6495D Triple Quadrupole and Evosep One;** Hoi-Ting Wu Quanrud<sup>1</sup>; Linfeng Wu<sup>2</sup>; Hao Qian<sup>1</sup>; Yanan Yang<sup>2</sup>; Benjamin Ta<sup>1</sup>; Jessica Chan<sup>1</sup>; Purva Ranjan<sup>1</sup>; Robert Zawada<sup>1</sup>; Philip Ma<sup>1</sup>; Yi (JIMMY) Zeng<sup>1</sup>; Bruce Wilcox<sup>1</sup>; <sup>1</sup>PrognomiQ Inc, San Mateo, CA; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- TP 044 **Analysis of 3-Hydroxy-myristic acid by LC-MS/MS in plasma samples of rats dosed with endotoxin;** Usha Mishra; <sup>1</sup>University of Minnesota, Minneapolis, MN
- TP 045 **A Simple and Sensitive LC-MS/MS Method for Quantification of 7 $\alpha$ -hydroxy-4-cholesten-3-one (C4) in Human Serum;** Aiping Zhu<sup>1</sup>; Tian-Sheng Lu<sup>1</sup>; Shuyu Hou<sup>1</sup>; <sup>1</sup>Medpace, Cincinnati, OH
- TP 046 **Method Optimization for Enhanced Quantification of CGRP in Human CSF by IA-LC-MS/MS to Support a Target Engagement Study with Fremanezumab;** Hang Zeng<sup>1,2</sup>; Fangteng Dai<sup>1,2</sup>; Jacki Jacki Rorabaugh<sup>1,3</sup>; Juline Bryson<sup>1,4</sup>; Hussein Hallak<sup>1,5</sup>; Thelma Angeles<sup>1,2</sup>; <sup>1</sup>Teva Pharmaceuticals, West Chester, PA; <sup>2</sup>Biomarker and Metabolism Analytics, West Chester, PA; <sup>3</sup>Translational Medicine, West Chester, PA; <sup>4</sup>Clinical Development, West Chester, PA; <sup>5</sup>DMPK, Netanya, Israel
- TP 047 **Sensitive Detection and Quantitation of Protein Components of the Complement Pathway;** Luis F Schachner<sup>1</sup>; Cong Wu<sup>1</sup>; Jianhui Zhu<sup>2</sup>; Tiffany Wong<sup>3</sup>; Tiffany Wu<sup>3</sup>; Racquel Corpuz<sup>3</sup>; Bill Meilandt<sup>3</sup>; Ryan Kelly<sup>3</sup>; Felix Yeh<sup>3</sup>; Anne Biever<sup>3</sup>; Jesse Hanson<sup>1</sup>; John Chen<sup>2</sup>; John Tran<sup>3</sup>; <sup>1</sup>Genentech, Inc., South San Francisco, CA; <sup>2</sup>NovaBioAssays, Boston, Massachusetts; <sup>3</sup>Genentech Inc, South San Francisco, CA

### DISEASE BIOMARKERS 048-062

- TP 048 **A Validated LC-MS/MS Method for Quantification of 3-Bromotyrosine in Patients with EoE;** Morgan Thomas<sup>1</sup>; Mac Gilliland<sup>1</sup>; <sup>1</sup>Furman University, Greenville, SC
- TP 049 **Utilization of a multi-omics integrative platform to analyze the inflamed gut tissue microenvironment;** Zohaib N. Khan<sup>1</sup>; Cristina C. Clement<sup>1</sup>; Laura Santambrogio<sup>1</sup>; <sup>1</sup>Weill Cornell Medicine, New York, NY
- TP 050 **Picogram Sensitivity of a novel deep proteomics platform with picogram sensitivity and its application in Alzheimer's disease;** Dan Liu<sup>1,2,3</sup>; Feifei Hu<sup>1,2,3</sup>; Xinyan Xie<sup>1,2,3</sup>; Junyi Wang<sup>1,2,3</sup>; Yuanyuan Peng<sup>1,2,3</sup>; Yonghao Zhang<sup>4</sup>; Xiehua Ouyang<sup>4</sup>; Shanshan Lv<sup>4</sup>; Yanting Meng<sup>4</sup>; Libing Wang<sup>4</sup>; Ziquan Cao<sup>4</sup>; Yi Wang<sup>4</sup>; Hao Wu<sup>4</sup>; Yan Zeng<sup>1,2,3</sup>; <sup>1</sup>Brain Science and Advanced Technology Institute, Wuhan University of Science and Technology, Wuhan, China; <sup>2</sup>Geriatric Hospital Affiliated to Wuhan University of Science and Technology, Wuhan, China; <sup>3</sup>School of Public Health, Wuhan University of Science and Technology, Wuhan, China; <sup>4</sup>Nanomics Biotechnology, Hangzhou, China
- TP 051 **Development of an effective biomarker panel for diabetic kidney disease progression by using a nanobinder assisted sample processing platform;** Ban Zhao<sup>1,2</sup>; Yonghao Zhang<sup>3</sup>; Xiehua Ouyang<sup>3</sup>; Yi Wang<sup>3</sup>; Hao Wu<sup>3</sup>; Yonghui Mao<sup>1,2</sup>; <sup>1</sup>Department of Nephrology, Beijing Hospital, Dongcheng District, China; <sup>2</sup>National Center for Gerontology, Institute of Geriatric Medicine, Chinese Academy of Medical Sciences, Dongcheng District, China; <sup>3</sup>Nanomics Biotechnology, Hangzhou, China
- TP 052 **Identification of tumor-marker gangliosides for early cancer detection: a mass spectrometry approach;** Rachel Culp-Hill<sup>1</sup>; Collin Hill<sup>1</sup>; Adele Blackler<sup>1</sup>; <sup>1</sup>AOA Dx, Boulder, CO
- TP 053 **Association of external exposome with metabolome in early childhood allergic diseases;** Ha Eun SONG<sup>1</sup>; Mi Jeong Kim<sup>1</sup>; Hyo Yeong Lee<sup>1</sup>; Su Jung Kim<sup>1</sup>; Hyun Ju Yoo<sup>1</sup>; <sup>1</sup>ASAN Medical center, SEOUL, South Korea
- TP 054 **QUANTITATIVE ANALYSIS BY LC-MS/MS OF THYROID HORMONE BIOMARKERS EXTRACTED FROM BLOOD COLLECTED WITH THE TASSO MICROSAMPLING DEVICE;** Chad D. Christianson<sup>1</sup>; Jason S. Watts<sup>1</sup>; Brooke I. Whitson<sup>1</sup>; Jennifer S. Zimmer<sup>1</sup>; <sup>1</sup>Alturas Analytics, Moscow, ID



## TUESDAY POSTERS

- TP 055 **Evaluating Bone Marrow Lipidomic Changes and Their Potential Association with Alzheimer's Disease;** Sarah G. Clark<sup>1</sup>; Amie M. Solosky<sup>1</sup>; Charles A. Schurman<sup>2</sup>; Kenneth A. Wilson<sup>2</sup>; Lisa M. Ellerby<sup>2</sup>; Birgit Schilling<sup>2</sup>; Erin S. Baker<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>2</sup>Buck Institute for Research on Aging, Novato, CA
- TP 056 **Exploring the critical role of doubly polyunsaturated phosphatidylethanolamines in the production of ferroptotic hydroperoxy lipid signals using HPLC/MS/MS;** Svetlana N. Samovich<sup>1, 2</sup>; Karolina Mikulska-Ruminska<sup>3</sup>; Haider H. Dar<sup>2</sup>; Yulia Y. Tyurina<sup>2</sup>; Vladimir A. Tyurin<sup>2</sup>; Austin B. Souryavong<sup>2</sup>; Alexander A. Kapralov<sup>2</sup>; Andrew A. Amoscato<sup>2</sup>; Ofer Beharier<sup>4</sup>; S. Ananth Karumanchi<sup>5</sup>; Claudette M. St Croix<sup>6</sup>; Xin Yang<sup>7</sup>; Theodore R. Holman<sup>8</sup>; Andrew P. VanDemark<sup>9</sup>; Yoel Sadovsky<sup>10, 11</sup>; Rama K. Mallampalli<sup>12</sup>; Sally E. Wenzel<sup>2</sup>; Wei Gu<sup>7, 13, 14</sup>; Yuri L. Bunimovich<sup>14</sup>; Ivet Bahar<sup>15</sup>; Valerian E. Kagan<sup>2, 16, 17, 18</sup>; Hülya Bayır<sup>1, 19</sup>; <sup>1</sup>Department of Pediatrics, Division of Critical Care and Hospital Medicine, Redox Health Center, Vagelos College of Physicians and Surgeons, Columbia University Irving Medical Center, New York, NY; <sup>2</sup>Department of Environmental and Occupational Health, Center for Free Radical and Antioxidant Health, School of Public Health, University of Pittsburgh, Pittsburgh, PA; <sup>3</sup>Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Torun, Poland; <sup>4</sup>Obstetrics and Gynecology Division, Hadassah Medical Center, Faculty of Medicine of the Hebrew University of Jerusalem, Jerusalem, Israel; <sup>5</sup>Department of Medicine, Cedars-Sinai Medical Center, Los Angeles, CA; <sup>6</sup>Department of Cell Biology, University of Pittsburgh, Pittsburgh, PA; <sup>7</sup>Institute for Cancer Genetics, and Herbert Irving Comprehensive Cancer Center, Vagelos College of Physicians and Surgeons, Columbia University, New York, NY; <sup>8</sup>Department of Chemistry and Biochemistry, University of California, Santa Cruz, CA; <sup>9</sup>Department of Biological Sciences, University of Pittsburgh, Pittsburgh, PA; <sup>10</sup>Magee-Womens Research Institute, Department of Obstetrics, Gynecology, and Reproductive Sciences, University of Pittsburgh, Pittsburgh, PA; <sup>11</sup>Department of Microbiology and Molecular Genetics, University of Pittsburgh, Pittsburgh, PA; <sup>12</sup>Department of Internal Medicine, The Ohio State University, Columbus, OH; <sup>13</sup>Department of Pathology and Cell Biology, Vagelos College of Physicians and Surgeons, Columbia University, New York, NY; <sup>14</sup>Department of Dermatology, University of Pittsburgh, Pittsburgh, PA; <sup>15</sup>Laufer Center for Physical and Quantitative Biology, Laufer Center, Z-5252, Stony Brook University, Stony Brook, New York; <sup>16</sup>Department of Radiation Oncology, University of Pittsburgh, Pittsburgh, PA; <sup>17</sup>Department of Chemistry, University of Pittsburgh, Pittsburgh, PA; <sup>18</sup>Department of Pharmacology and Chemical Biology, University of Pittsburgh, Pittsburgh, PA; <sup>19</sup>Department of Critical Care Medicine, Safar Center for Resuscitation Research, Children's Neuroscience Institute, Children's Hospital of Pittsburgh, University of Pittsburgh, Pittsburgh, PA
- TP 057 **Phosphoproteomics predict response to Venetoclax plus Azacitidine in Acute Myeloid Leukemia patients;** Josie A. Christopher<sup>1</sup>; Luis Nobre<sup>1</sup>; Weronika E. Borek<sup>1</sup>; Amy E. Campbell<sup>1</sup>; David N. Perkins<sup>1</sup>; Pedro Moreno-Cardoso<sup>1</sup>; Nazrath Nawaz<sup>1</sup>; Janet Kelsall<sup>1</sup>; Paolo Gallipoli<sup>2</sup>; Andrea Arruda<sup>3</sup>; Alex Ambinder<sup>4</sup>; Andrew Thompson<sup>1</sup>; Andrew Williamson<sup>1</sup>; Gabriel Ghiaur<sup>4</sup>; Sayantane Datta<sup>5</sup>; Mark D. Minden<sup>3, 6</sup>; David J. Britton<sup>1</sup>; Heinz Sill<sup>7</sup>; John G. Gribben<sup>2</sup>; Pedro R. Cutillas<sup>1, 2</sup>; Arran D. Dokal<sup>1</sup>; <sup>1</sup>Kinomica Ltd, Macclesfield, Cheshire, United Kingdom; <sup>2</sup>Barts Cancer Institute, Queen Mary University of London, London, United Kingdom; <sup>3</sup>Princess Margaret Cancer Centre, University Health Network, Toronto, ON; <sup>4</sup>Johns Hopkins Sidney Kimmel Comprehensive Cancer Center, Baltimore, MD; <sup>5</sup>Division of Hematology, Medical University of Graz, Graz, Austria; <sup>6</sup>Department of Medical Biophysics, University of Toronto, Toronto, ON
- TP 058 **Paramagnetic Bead-Based Multi-Omics Profiling of Human Serum in Alzheimer's Disease;** Ching-Yuan Yang<sup>1</sup>; Haiyan Lu<sup>2</sup>; Michael M. Rosenblatt<sup>3</sup>; Lingjun Li<sup>2, 4</sup>; <sup>1</sup>Biophysics Graduate Program, University of Wisconsin-Madison, Madison, Wisconsin; <sup>2</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin; <sup>3</sup>Promega Corporation, Madison, Wisconsin; <sup>4</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin
- TP 059 **Unveiling Proteomic Signatures of Tau Pathogenesis through Label-Free Mass Spectrometry Analysis;** Xuemei Zeng<sup>1</sup>; Yijun Chen<sup>1</sup>; Anuradha Sehwari<sup>1</sup>; Eric E. Abrahamson<sup>1, 2</sup>; Julia K. Kofler<sup>1</sup>; William R. Paljug<sup>1, 2</sup>; Miloslav D. Ikonovic<sup>1, 2</sup>; Thomas K. Karikari<sup>1</sup>; <sup>1</sup>University of Pittsburgh, Pittsburgh, PA; <sup>2</sup>VA Pittsburgh Healthcare System, Pittsburgh, Pennsylvania
- TP 060 **Investigation of blood proteomic biomarkers in individuals with Nieman-Pick Disease Type C1;** Olivia C Wagner<sup>1</sup>; Wenping Li<sup>1</sup>; Derek Alexander<sup>2</sup>; Forbes D. Porter<sup>2</sup>; Stephanie M. Cologna<sup>3</sup>; <sup>1</sup>University of Illinois Chicago, Chicago, IL; <sup>2</sup>NIH, Bethesda, MD; <sup>3</sup>University of Illinois at Chicago, Chicago, IL
- TP 061 **Development of a targeted multiplexed method to measure complement activation in human ocular samples;** Yadira X Perez Paramo<sup>1</sup>; Erin Tom<sup>1</sup>; Shelby M Coates<sup>2</sup>; Michael C Chang<sup>1</sup>; Lee A Honigberg<sup>1</sup>; W Rodney Mathews<sup>1</sup>; Veronica G Anania<sup>1</sup>; <sup>1</sup>Genentech, South San Francisco, CA; <sup>2</sup>Washington State University, Spokane, WA
- TP 062 **Defining the proteome, glycoproteome and lipidome by mass spectrometry in a congenital disorder of glycosylation for discovering diagnostic biomarkers;** Anu Jain<sup>1</sup>; Kishore Garapati<sup>1</sup>; Seul Kee Byeon<sup>1</sup>; Rohit Budhraj<sup>1</sup>; Wasantha Ranatunga<sup>1</sup>; Christina Lam<sup>2, 3</sup>; Matthew J. Schultz<sup>1</sup>; Tamas Kozicz<sup>1, 4, 5</sup>; Eva Morava<sup>1, 4, 5</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN; <sup>2</sup>Seattle Children's Research Institute, Seattle, United Kingdom; <sup>3</sup>University of Washington School of Medicine, Seattle, Washington; <sup>4</sup>Icahn School of Medicine at Mount Sinai, New York, NY; <sup>5</sup>University of Pecs Medical School, Pecs, Hungary

### ENVIRONMENTAL: GENERAL II 063-098

- TP 063 **Putative Identification of Hydroxyproline-containing Microcystins by UHPLC-MS/MS;** Sanduni H Premathilaka<sup>1</sup>; Judy A Westrick<sup>2</sup>; Dragan Isailovic<sup>1</sup>; <sup>1</sup>University of Toledo, Toledo, OH; <sup>2</sup>Wayne State University, Detroit, MI
- TP 064 **Novel Separation Method of Per- and Polyfluoroalkyl Substances Via 2D LCxDMs-MS2;** Christopher Ryan<sup>1</sup>; Emir Nazdrajić<sup>1</sup>; J. Larry Campbell<sup>2</sup>; W. Scott Hopkins<sup>1, 3, 4</sup>; <sup>1</sup>University of Waterloo, Waterloo, ON; <sup>2</sup>Bedrock Scientific Inc, Milton, ON; <sup>3</sup>Watermine Innovation, Waterloo, ON; <sup>4</sup>Centre for Eye and Vision Research, Hong Kong, Hong Kong
- TP 065 **Analytical Characterization of Cannabis Flower Buds by LC-MS and ICP-MS;** Kingsley K Donkor<sup>1</sup>; Nicole Hanna<sup>1</sup>; Devansh Sharma<sup>1</sup>; Tharusha Jayasinghe<sup>1</sup>; <sup>1</sup>Thompson Rivers University, Kamloops, BC
- TP 066 **Investigation of Thermal Decomposition Poly-Fluoroalkyl Substances (PFAS) with Thermal Desorption - Pyrolysis - Gas Chromatography-Mass Spectrometry;** Katerina Litvanova<sup>1</sup>; Bethany Klemetsrud<sup>2</sup>; Feng Xiao<sup>3</sup>; Alena Kubatova<sup>1</sup>; <sup>1</sup>University of North Dakota, Grand Forks, ND; <sup>2</sup>Department of Chemical Engineering, University of North Dakota, Grand Forks, ND; <sup>3</sup>University of Missouri-Columbia, Columbia, MO
- TP 067 **Quantification of Brominated Flame Retardants in Polymer Samples Using Direct Mass Spectrometric Analysis;** Krista Grönlund<sup>1</sup>; Ville Nissinen<sup>1</sup>; Kirsi Korpijärvi<sup>2</sup>; Milad Mosallaei<sup>3</sup>; Ilkka Rytöluoto<sup>3</sup>; Jani Pelto<sup>3</sup>; Mika Suvanto<sup>1</sup>; Jarkko J. Saarinen<sup>1</sup>; Janne Jänis<sup>1</sup>; <sup>1</sup>University of Eastern Finland, JOENSUU, Finland; <sup>2</sup>VTT Technical

## TUESDAY POSTERS

- Research Centre of Finland Ltd., Jyväskylä, Finland; <sup>3</sup>VTT Technical Research Centre of Finland Ltd., Tampere, Finland
- TP 068 **Automated targeted and non-targeted LC-Orbitrap MS workflow for analysis of more than 40,000 PFAS compounds;** Cynthia M Grim<sup>1</sup>; Toby Astill<sup>1</sup>; Valérie Thibert<sup>2</sup>; Aristide Ganci<sup>2</sup>; Bénédicte Gauriat<sup>2</sup>; Richard Cochran<sup>3</sup>; P Lee Ferguson<sup>4</sup>; Jean-François Garnier<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Courtaboeuf, France; <sup>3</sup>Thermo Fisher Scientific, Bannockburn, IL; <sup>4</sup>Department of Civil and Environmental Engineering and Nicholas School of the Environment, Duke University, Durham, NC
- TP 069 **Real Time Monitoring of Semi-Volatile Emerging Atmospheric Contaminants: Application of the AIM Reactor in PFAS Detection;** Omar El Hajj<sup>1</sup>; Spiro Jorga<sup>2</sup>; Abigail Koss<sup>1</sup>; Veronika Pospisilova<sup>2</sup>; Wade Bontempo<sup>1</sup>; Joel Kimmel<sup>1</sup>; <sup>1</sup>Tofwerk USA, Boulder, CO; <sup>2</sup>TOFWERK AG, Thun, Switzerland
- TP 070 **Cyanobacterial classification using a DART-Orbitrap mass spectrometer;** Yuya Takai<sup>1</sup>; Wakana Hosoe<sup>2</sup>; Yuka Tsuboi<sup>2</sup>; Shunichi Ishikawa<sup>2</sup>; Hana Kozaki<sup>2</sup>; Masaki Hoshino<sup>2</sup>; Masahiko Tachi<sup>3</sup>; Hajime Mizuno<sup>2</sup>; Susumu Y. Imanishi<sup>2</sup>; <sup>1</sup>Meijo University, Nagoya, Japan; <sup>2</sup>Meijo University, Nagoya, Japan; <sup>3</sup>Aichi Prefectural Institute of Public Health, Nagoya, Japan
- TP 071 **Association between plasma metabolites and heavy metal exposure in residents of environmentally polluted areas;** Mi Jeong Kim<sup>1</sup>; Ha Eun SONG<sup>1</sup>; Hyo Yeong Lee<sup>1</sup>; Su Jung Kim<sup>1</sup>; Hyun Ju Yoo<sup>1</sup>; <sup>1</sup>ASAN Medical center, SEOUL, South Korea
- TP 072 **Point-of-Use Activated Carbon Filters Reduce Calculated Cyto- and Genotoxicity of Drinking Water by Removal of Regulated and Unregulated Disinfection Byproducts;** Erin Katie Jaynes<sup>1</sup>; Patrick T Justen<sup>1</sup>; Amy A Cuthbertson<sup>1</sup>; Ashley A Perkins<sup>1</sup>; Vincent Esposito<sup>1</sup>; Hannah K Liberatore<sup>1</sup>; Susan D Richardson<sup>1</sup>; <sup>1</sup>University of South Carolina, Columbia, SC
- TP 073 **Analysis of PFAS and other environmental contaminants in soil and oat plants using high resolution GC/MS;** Sofia Nieto<sup>1</sup>; Matthew Giardina<sup>1</sup>; Matthew Curtis<sup>1</sup>; Luann Wong<sup>2</sup>; Gabrielle Black<sup>2</sup>; Thomas Young<sup>2</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>University of California, Davis, Davis, CA
- TP 074 **Studies of the adsorption process of organic pollutants on microplastics using high-throughput SPME-MOI-LEI-MS;** Tommaso Grazioso<sup>1</sup>; Adriana Arigò<sup>1</sup>; Giorgio Famigliini<sup>1</sup>; Pierangela Palma<sup>1,2</sup>; ACHILLE CAPPIELLO<sup>1,2</sup>; <sup>1</sup>Università degli studi di Urbino Carbo Bo, Urbino, Italy; <sup>2</sup>Vancouver Island University, Nanaimo, BC
- TP 075 **Faster Analysis for Forever Chemicals: Accelerating PFAS Analysis with UPLC-HRIM-MS;** Alan McKenzie-Coe<sup>1</sup>; Thomas Lubinsky<sup>1</sup>; Jeremy P. Koelmel<sup>2</sup>; Emma E. Rennie<sup>3</sup>; David A Weil<sup>3</sup>; Sarah M. Stow<sup>3</sup>; Paul Stelben<sup>2</sup>; Krystal J. Godri Pollitt<sup>4</sup>; David Godri<sup>5</sup>; Frederick Strathmann<sup>1</sup>; Daniel DeBord<sup>6</sup>; <sup>1</sup>MOBILion Systems, Chadds Ford, PA; <sup>2</sup>Innovative Omics, Sarasota, FL; <sup>3</sup>Agilent Technologies, Santa Clara, CA; <sup>4</sup>Yale University, New Haven, CT; <sup>5</sup>3rd Floor Solutions, Toronto, Ontario; <sup>6</sup>MOBILionSystems, Chadds Ford, PA
- TP 076 **Systematic Study of Techniques to Minimize PFAS Background Interferences;** Om K Shrestha<sup>1</sup>; Kathleen K Luo<sup>1</sup>; Megan Davis<sup>1</sup>; Landon A Wiest<sup>1</sup>; Evelyn H Wang<sup>1</sup>; Xiaomeng Xia<sup>1</sup>; Keith Herman<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD
- TP 077 **Complementary Quantitative and Qualitative Mass Spectrometry Analysis for Environmental Samples;** Kendra Selby<sup>1</sup>; Stephanie Shan<sup>1</sup>; Summy Shrestha<sup>1</sup>; Claire Korte<sup>1</sup>; M Nazim Boutaghou<sup>2</sup>; Samantha A Olendorff<sup>2</sup>; Kevin R Tucker<sup>1</sup>; <sup>1</sup>Southern Illinois University Edwardsville, Edwardsville, IL; <sup>2</sup>Shimadzu Scientific Instruments, Columbia, MD
- TP 078 **Physicochemical Properties and Partitioning Behaviour of para-Phenylenediamine quinones (PPDQs) Investigated with Direct Mass Spectrometry;** Misha Zvejkic<sup>1,2</sup>; Joseph Monaghan<sup>1,2</sup>; Angelina Jaeger<sup>1,2</sup>; Chris G Gill<sup>1,2,3,4</sup>; Erik T Krogh<sup>1,2</sup>; <sup>1</sup>Vancouver Island University, Nanaimo, BC; <sup>2</sup>University of Victoria, Victoria, BC; <sup>3</sup>Simon Fraser University, Burnaby, BC; <sup>4</sup>University of Washington, Seattle, WA
- TP 079 **Extraction Optimization and Non-Targeted Analyses of Per- and Polyfluoroalkyl Substances (PFAS) in Mammalian Milk;** Kara M Joseph<sup>1</sup>; Gregory Kudzin<sup>1</sup>; Anna K. Boatman<sup>1</sup>; Erin S. Baker<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 080 **Classification and identification of cyanobacteria in frozen samples using MALDI Biotyper;** Sakura Kawasaki<sup>1</sup>; Haruka Okuma<sup>1</sup>; Takahiro Wakayama<sup>1</sup>; Kosuke Hatanaka<sup>1</sup>; Yuka Maruoka<sup>1</sup>; Hajime Mizuno<sup>1</sup>; Susumu Y. Imanishi<sup>1</sup>; <sup>1</sup>Meijo University, Nagoya, Japan
- TP 081 **Photoionization High-Resolution Mass Spectrometry for Analysis of Atmospheric Particulate Matter;** Hendryk Czech<sup>1,2</sup>; Patrick Martens<sup>1</sup>; Sven Ehler<sup>3</sup>; Paul Kösling<sup>1</sup>; Marco Schmidt<sup>1</sup>; Christopher Rürger<sup>1</sup>; Johannes Passig<sup>1,2</sup>; Thorsten Streibel<sup>1,2</sup>; Martin Rigler<sup>4</sup>; Andreas Walte<sup>3</sup>; Ralf Zimmermann<sup>1,2</sup>; <sup>1</sup>University of Rostock, Rostock, Germany; <sup>2</sup>Joint Mass Spectrometry Centre, Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Munich, Munich, Germany; <sup>3</sup>Photonion GmbH, Schwerin, Germany; <sup>4</sup>Aerosol Magee Inc., Ljubljana, Slovenia
- TP 082 **New approach for assigning emerging contaminants from high-resolution mass spectrometry data – comprehensive screening and Kendrick mass defect network analysis;** Laura Tenhumberg<sup>1</sup>; Alessandro Vetere<sup>2</sup>; Wolfgang Schrader<sup>2</sup>; <sup>1</sup>Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany; <sup>2</sup>Max-Planck-Institut für Kohlenforschung, 45470 Mülheim an der Ruhr, Germany
- TP 083 **Comprehensive identification of toxic chemicals in road marking paint using integrated pyrolysis-GC-MS, GC-MS, LC-MS/MS, and ICP-MS analysis;** Seungwoo Seo<sup>1</sup>; Tae-Young Kim<sup>1</sup>; <sup>1</sup>School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea
- TP 084 **Unveiling the hidden threat: Paint microplastics and their extractable organics in soil;** Woo-Young Song<sup>1</sup>; Shin Woong Kim<sup>2,3</sup>; Walter R. Waldman<sup>4</sup>; Matthias C. Rillig<sup>2,3</sup>; Tae-Young Kim<sup>1</sup>; <sup>1</sup>School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea; <sup>2</sup>Institute of Biology, Freie Universität Berlin, Berlin, Germany; <sup>3</sup>Berlin-Brandenburg Institute of Advanced Biodiversity Research, Berlin, Germany; <sup>4</sup>Science and Technology Center for Sustainability, Federal University of São Carlos, São Carlos, Brazil
- TP 085 **Detecting PFAS beyond the Current Regulatory Request: a Comprehensive Overview of the Contamination in Water by UPHLC-Ion mobility-HRMS;** Arnd Ingendoh<sup>1</sup>; Igor Nikitin<sup>1</sup>; Carsten Baessmann<sup>1</sup>; Andrea Kiehne<sup>1</sup>; Eva-Maria Niehaus<sup>1</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany
- TP 086 **Evaluation of DESI mounted on Q-ToF and TQ mass spectrometers to image PFAS compounds in different matrices;** Emmanuelle Claude<sup>1</sup>; Alexandra Lee<sup>1</sup>; Mujeebatu Kadiri-Asamoah<sup>1</sup>; Stuart Adams<sup>1</sup>; Emrys Jones<sup>1</sup>; Joanne Ballantyne<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom
- TP 087 **Untargeted Screening for PFAS Chemicals Using Comprehensive Feature Detection;** Jeff Goshawk<sup>1</sup>; Andrew Tudor<sup>1</sup>; Sarah Dowd<sup>2</sup>; Jonathan Fox<sup>1</sup>; Hania Khoury-Hollins<sup>1</sup>; Michael McCullagh<sup>1</sup>; Isabel Riba<sup>1</sup>; Susan Slade<sup>1</sup>; Russell Mortshire-Smith<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Waters Corporation, Milford, Massachusetts

- TP 088 **Identification of short chain per and polyfluorinated alkyl substances (PFAS) using ion ratios with low mass product ions;** Kieron Faherty<sup>1</sup>; Stuart J Adams<sup>2</sup>; Kate Whyatt<sup>2</sup>; David Gordon<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, Massachusetts; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom
- TP 089 **A novel approach to identifying Environmental Risk Factors for Breast Cancer Through Integrated Untargeted and Targeted HSA Adductomics;** Fariba Tayyari<sup>1</sup>; Aishwarya Jala<sup>1</sup>; Yeunook Bae<sup>1</sup>; Cathelin Huang<sup>1</sup>; James Burke<sup>1</sup>; Kwang-Youn Kim<sup>1</sup>; Kalliopi Siziopikou<sup>1</sup>; Alexander White<sup>2</sup>; Dale Sandler<sup>2</sup>; William E Funk<sup>1</sup>; <sup>1</sup>Northwestern University, Chicago, IL; <sup>2</sup>NIH/NIEHS, Research Triangle Park, NC
- TP 090 **Expanding the known chemical universe for vehicle tire related emerging contaminants with complementary non-targeted analysis (NTA) approaches;** Mauricio Marques Dos Santos<sup>1</sup>; Isaac Wai Loon Law<sup>1</sup>; Shane Allen Snyder<sup>1</sup>; <sup>1</sup>Nanyang Technological University (NTU)- NEWRI, Singapore, Singapore
- TP 091 **Analysis of PFAS in Potable Water by Direct Injection Using the LCMS-8060NX;** Luis O Junqueira<sup>1</sup>; Marcos A Pudenzi<sup>1</sup>; Lucas L Zanin<sup>1</sup>; Ichiro Hirano<sup>1</sup>; <sup>1</sup>Shimadzu do Brasil, Barueri, Brazil
- TP 092 **Characterization of PFAS chemicals in anti-fog solutions using gas chromatography and high-performance time-of-flight mass spectrometry;** Katie Redinius<sup>1</sup>; David E Alonso<sup>2</sup>; Joe Binkley<sup>1</sup>; <sup>1</sup>LECO Corporation, Saint Joseph, MI; <sup>2</sup>Leco Corporation, St. Joseph, MI
- TP 093 **Analysis of PFAS in water using Head-Space Solid Phase Microextraction-Gas Chromatography/Mass Spectrometry (HS-SPME GCMS);** Andy Sandy<sup>1</sup>; Evelyn Wang<sup>1</sup>; Yoshiyuki Okamura<sup>1</sup>; Ruth Marfil-Vega<sup>1</sup>; Alan Owens<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD
- TP 094 **Expanding Molecular Compositional Coverage of Water-Soluble Emerging Contaminants with Liquid Chromatography – Ultrahigh-Resolution Mass Spectrometry;** Joseph W. Frye-Jones<sup>1,2</sup>; Martha L. Chacon-Patino<sup>1,3</sup>; Lissa C. Anderson<sup>1</sup>; Alvaro J. Tello-Rodriguez<sup>1,4</sup>; Winston K. Robbins<sup>1</sup>; Alan G. Marshall<sup>1,2</sup>; Ryan P. Rodgers<sup>1,2,3,5</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, Florida; <sup>2</sup>Florida State University - Department of Chemistry and Biochemistry, Tallahassee, FL; <sup>3</sup>International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France; <sup>4</sup>Florida State University, Tallahassee, FL; <sup>5</sup>Université de Pau et des Pays de l'Adour, Pau, France
- TP 095 **Simultaneous Identification and Quantification of Lignin Breakdown Products by Thermal Desorption Pyrolysis Gas Chromatography Mass Spectrometry Methanizer Flame Ionization Detector;** Mason L Clobes<sup>1</sup>; Md Musfiqur Rahman<sup>1,2</sup>; Nafisa Bala<sup>1</sup>; Alena Kubatova<sup>1</sup>; <sup>1</sup>University of North Dakota, Grand Forks, ND; <sup>2</sup>Winder Laboratories, Winder, GA
- TP 096 **Peekaboo, PFAS in fabrics and textiles, we see you;** Zijie Xia<sup>1</sup>; Sawyer Schugel<sup>1</sup>; Pheng Yang<sup>1</sup>; Brian Beall<sup>1</sup>; <sup>1</sup>Claros Technologies, Minneapolis, MN
- TP 097 **Optimizing Orbitrap-based isotopic analysis of nitrate by coupling Orbitrap-MS with chromatographic separation techniques;** Allyson Girard<sup>1</sup>; Justin Y Elliott<sup>1</sup>; J. David Felix<sup>1</sup>; Hussain Abdulla<sup>1</sup>; <sup>1</sup>Texas A&M University-Corpus Christi, Corpus Christi, TX
- TP 098 **Investigating electron shuttling within the dissolved organic matter pool of an Iron-oxidizing microbial community using high-resolution Tandem Mass Spectrometry;** Tilman Schramm<sup>1</sup>; Cristina Escudero Parada<sup>2</sup>; Paolo Stincone<sup>2</sup>; Abzer Shah<sup>2</sup>; Franziska Schädler<sup>2</sup>; Lars Grimm<sup>2</sup>; Marie Mollenkopf<sup>2</sup>; Verena Nikeleit<sup>2</sup>; Andreas Kappler<sup>2</sup>; Daniel Petras<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA; <sup>2</sup>University of Tuebingen, Germany, Tuebingen, Germany
- TP 099 **The Exposome Posits a Cause for Cancer: Assessing the Hemoglobin Adductome of a Multi-Ethnic Cohort of Smokers by Targeted LC/MS;** Erik J Moran<sup>1</sup>; Yuliet Monatikwa<sup>1</sup>; Allysha O'Donnell<sup>1</sup>; Abdur Rahim<sup>1</sup>; Andrew Rajczewski<sup>1</sup>; Joshua Gann<sup>1,2</sup>; Alexander Hurben<sup>1,3</sup>; Gunnar Boysen<sup>4</sup>; Natalia Tretyakova<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>Vanderbilt University, Nashville, TN; <sup>3</sup>University of California, Berkeley, Berkeley, CA; <sup>4</sup>University of Arkansas for Medical Sciences, Little Rock, AR
- TP 100 **The chemical exposome in glioblastoma and its potential connection with ultrafine particles;** Ruben Gil-Solsona<sup>1,2</sup>; Daniel Gutierrez-Martin<sup>1</sup>; Albert Pons-Escoda<sup>3,4</sup>; Carles Majos<sup>3,4</sup>; Noemi Vidal<sup>4,5</sup>; Fulvio Amato<sup>1</sup>; Gunnar Christina Nika<sup>1</sup>; Pablo Gago Ferrero<sup>6</sup>; <sup>1</sup>IDAEA-CSIC, Barcelona, Spain; <sup>2</sup>National and Kapodistrian University of Athens Medical School, Athens, Greece; <sup>3</sup>Radiology Department, Hospital Universitari de Bellvitge, Barcelona, Spain; <sup>4</sup>Neuro-Oncology Unit, Institut d'Investigació Biomedica de Bellvitge, IDIBELL, Barcelona, Spain; <sup>5</sup>Department of Pathology, Hospital de Bellvitge, Barcelona, Spain; <sup>6</sup>Institute of Environmental Assessment and Water Research - Spanish Council for Scientific Research (IDAEA-CSIC), Barcelona, Spain
- TP 101 **An Assessment of Serum Lipidomic Perturbations due to Drinking Water and Occupational PFAS Exposures;** Ashlee T Falls<sup>1</sup>; Anna K. Boatman<sup>2</sup>; Kaylie I Kirkwood-Donelson<sup>3</sup>; Heather M. Stapleton<sup>4</sup>; Erin S. Baker<sup>2</sup>; <sup>1</sup>University of North Carolina - Chapel Hill, Chapel Hill, NC; <sup>2</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>3</sup>National Institute of Environmental Health Sciences, Durham, NC; <sup>4</sup>Duke University, Durham, NC
- TP 102 **A Multidimensional Database for the Detection of Quaternary Ammonium Compounds and Their Phase I Metabolites in Humans;** Ryan Nguyen<sup>1</sup>; Ryan P. Seguin<sup>1</sup>; Dylan H. Ross<sup>2</sup>; Pengyu Chen<sup>1</sup>; Sean H. Richardson<sup>3</sup>; Jennifer Liem<sup>4</sup>; Yvonne S. Lin<sup>4</sup>; Libin Xu<sup>1</sup>; <sup>1</sup>Department of Medicinal Chemistry, University of Washington, Seattle, WA; <sup>2</sup>Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; <sup>3</sup>Department of Mathematics, University of Washington, Seattle, WA; <sup>4</sup>Department of Pharmaceutics, University of Washington, Seattle, WA
- TP 103 **Evaluating Environmental Factors in Systemic Autoimmune Rheumatic Diseases with Non-Targeted Analyses of Patients and Their Unaffected Siblings;** Gregory Kudzin<sup>1</sup>; James N. Dodds<sup>1</sup>; Kaylie I. Kirkwood-Donelson<sup>2</sup>; Adam Schifffenbauer<sup>3</sup>; Frederick W. Miller<sup>3</sup>; Kakali Sarkar<sup>3</sup>; Payam Noroozi Farhadi<sup>3</sup>; Alan K. Jarmusch<sup>4</sup>; Lisa G. Rider<sup>3</sup>; Erin S. Baker<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>2</sup>National Institute of Environmental Health Sciences, Durham, NC; <sup>3</sup>Environmental Autoimmunity Group, Clinical Research Branch, National Institute of Environmental Health Sciences, Bethesda, MD; <sup>4</sup>Immunity, Inflammation, and Disease Laboratory, National Institute of Environmental Health Sciences, Durham, NC
- TP 104 **Evaluating Ion Mobility (IM) and Multi Reflecting Time-of-Flight (MRT) Mass Spectrometry Platforms for Non-targeted LC-MS, LC-MS/MS and LC-IM-MS Exposomic Studies;** David C Koomen<sup>1</sup>; Jody C May<sup>1</sup>; Katrina L Leaptrot<sup>1</sup>; Alexandra C Rutledge-Schrimpe<sup>1</sup>; Simona G Codreanu<sup>1</sup>; Jerry D Holman<sup>1</sup>; Hania Khoury-Hollins<sup>2</sup>; Lee A Gethings<sup>2</sup>; Stacy D Sherrod<sup>1</sup>; John A McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom
- TP 105 **Characterization of reactive electrophiles-derived exposome by profiling urinary mercapturic acid conjugates using enzymatic deacetylation and data-independent acquisition mass spectrometry;** Yuan-Chih Chen<sup>1</sup>; Pao-Chi Liao<sup>1</sup>; <sup>1</sup>National Cheng Kung University, Tainan, Taiwan

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- TP 106 **Discovery of Noninvasive Biomarkers for Radiation Exposure via LC-MS-based Hair Metabolomics;** Huan Zhang<sup>1,2</sup>; Rui Xui<sup>1,2</sup>; Shruthi Kandalai<sup>1,3,4</sup>; Haidong Peng<sup>1,3,4</sup>; Michael Geiman<sup>1,3</sup>; Shuaixin Gao<sup>1,2</sup>; Naduparambil K. Jacob<sup>1,3</sup>; Qingfei Zheng<sup>1,3,4</sup>; Jiangjiang Zhu<sup>1,2</sup>; <sup>1</sup>Comprehensive Cancer Center, The Ohio State University, Columbus, OH, 43210; <sup>2</sup>Human Nutrition Program, Department of Human Sciences, The Ohio State University, Columbus, OH, 43210; <sup>3</sup>Department of Radiation Oncology, College of Medicine, The Ohio State University, Columbus, OH, 43210; <sup>4</sup>Center for Cancer Metabolism, The Ohio State University, Columbus, OH, 43210
- TP 107 **A mass spectrometry-based scalable workflow for exposome research;** Xiangping Lin<sup>1</sup>; Xinyue Zhang<sup>1</sup>; Michael P. Snyder<sup>1</sup>; <sup>1</sup>Department of Genetics, Stanford University School of Medicine, Stanford, CA
- TP 108 **Label-free protein expression analysis from mammalian tissues following dermal exposure to perfluorobutanoic acid;** Madison P. Cooper<sup>1</sup>; Stacey E. Anderson<sup>1</sup>; Lisa M. Weatherly<sup>1</sup>; Laurel G. Jackson<sup>1</sup>; Ewa Lukomska<sup>1</sup>; Justin M. Hettick<sup>1</sup>; <sup>1</sup>NIOSH, Morgantown, WV
- TP 109 **Assessment of exposure to oxybenzone, synthetic antioxidants and triclosan using targeted and untargeted LC-MS/MS of urine samples;** Said Matar<sup>1,2</sup>; Lekha Sleno<sup>1,2</sup>; <sup>1</sup>University of Quebec in Montreal, Montreal, QC; <sup>2</sup>Ecotox research network on ecotoxicology research, Montreal, QC
- TP 110 **Hair as a high-value matrix for exposomics: multi-residue analysis of xenobiotics by LC-HRMS;** Delia Castilla-Fernández<sup>1</sup>; Benedikt Warth<sup>1</sup>; <sup>1</sup>University of Vienna, Department of Food Chemistry and Toxicology, Faculty of Chemistry, Vienna, Austria., Vienna, Austria
- TP 111 **Enhanced Coverage of volatile and semi-volatile PFAS Using Experimental and Predicted GC-HRMS PCI and EI libraries;** Jeremy Koelmel<sup>1</sup>; Elizabeth Z. Lin<sup>1</sup>; Emily Johnson<sup>1</sup>; Paul Stelben<sup>1</sup>; Sheng Liu<sup>1</sup>; Kozo Nishida<sup>2</sup>; Hiroshi Tsugawa<sup>2</sup>; Ashley Lin<sup>3,4</sup>; Yakun Zhou<sup>1</sup>; Vladimir Nikiforov<sup>5</sup>; Alexander Aksenov<sup>6</sup>; Joseph Okeme<sup>1</sup>; John Bowden<sup>1</sup>; Krystal Godri Pollitt<sup>1</sup>; <sup>1</sup>Yale University, New Haven, CT; <sup>2</sup>Tokyo University of Agriculture and Technology, Koganei-shi, Japan; <sup>3</sup>University of Florida, Gainesville, FL; <sup>4</sup>University of Florida, GAINESVILLE, FL; <sup>5</sup>NILU, Kjeller, Norway; <sup>6</sup>University of Connecticut, Storrs, CT; <sup>7</sup>University of Florida Department of Chemistry, Gainesville, FL
- TP 112 **Urine metabolomics analysis of dermal exposure to spray polyurethane foam;** Chani Sahabandu Hewa Sahabanduge<sup>1</sup>; Kushal Biswas<sup>1</sup>; Dhimiter Bello<sup>1</sup>; Pengyuan Liu<sup>2</sup>; <sup>1</sup>University of Massachusetts Lowell, Lowell, MA; <sup>2</sup>University of Massachusetts, Lowell, Lowell, MA
- TP 113 **Leveraging the MS1 Dimension and Formula Prediction in Non-Targeted Analysis of PFAS using New FluoroMatch Algorithms: Assessing Confidence and Coverage;** David Schiessel<sup>1</sup>; Jeremy Koelmel<sup>2</sup>; Michael Kummer<sup>1</sup>; David Godri<sup>3</sup>; Sheng Liu<sup>2</sup>; Elizabeth Z. Lin<sup>2</sup>; John Bowden<sup>4</sup>; Olivier Chevallier<sup>5</sup>; Camden G. Camacho<sup>4</sup>; Emma Rennie<sup>2</sup>; Krystal Godri Pollitt<sup>2</sup>; <sup>1</sup>Innovative Omics, Sarasota, FL; <sup>2</sup>Yale University, New Haven, CT; <sup>3</sup>3rd Floor Solutions, Toronto, Ontario; <sup>4</sup>University of Florida, Gainesville, FL; <sup>5</sup>Agilent Technologies, Santa Clara, CA
- TP 114 **MRM-profiling for detecting emerging contaminants in human biomonitoring: Application to Bisphenol A replacements;** Jasmin Chovatiya<sup>1</sup>; Ravikumar Jagani<sup>1</sup>; Manish Arora<sup>1</sup>; Syam S. Andra<sup>1</sup>; <sup>1</sup>Institute for Exposomic Research, Department of Environmental Medicine and Public Health, New York, NY
- TP 115 **Evaluating Lipidomic Changes in Mice Exposed to Wildfire-Relevant Smoke from Different Fuel and Burn Conditions;** Haley C. Jostes<sup>1</sup>; Amie M. Solosky<sup>1</sup>; Jessie R. Chappel<sup>2</sup>; Celeste Carberry<sup>1</sup>; Julia E. Rager<sup>1</sup>; Erin S. Baker<sup>1</sup>; <sup>1</sup>UNC-Chapel Hill, Chapel Hill, NC; <sup>2</sup>North Carolina State University, Raleigh, NC
- TP 116 **A Lipidomic Exploration of the Impact of Perfluorooctanoic Acid (PFOA) Exposure on SARS-CoV-2 Infection;** Allison N. Fry<sup>1</sup>; Jessie R. Chapel<sup>2</sup>; Amie M. Solosky<sup>1</sup>; Kara M. Joseph<sup>1</sup>; Sarah G. Clark<sup>1</sup>; Deanna Lanier<sup>3</sup>; Mario Uchimiya<sup>3</sup>; Dawne Rowe<sup>4</sup>; David A. Gaul<sup>5</sup>; Facundo M. Fernandez<sup>5</sup>; S. Mark Tompkins<sup>4</sup>; Tracey Woodlief<sup>6</sup>; Jamie DeWitt<sup>7</sup>; Arthur Edison<sup>3</sup>; Erin S. Baker<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>2</sup>Bioinformatics Research Center, Department of Biological Sciences, North Carolina State University, Raleigh, NC; <sup>3</sup>Complex Carbohydrate Research Center, University of Georgia, Athens, GA; <sup>4</sup>Center for Vaccines and Immunology, University of Georgia, Athens, GA; <sup>5</sup>School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; <sup>6</sup>Department of Pharmacology and Toxicology, Brody School of Medicine, East Carolina University, Greenville, NC; <sup>7</sup>Department of Environmental and Molecular Toxicology, Oregon State University, Corvallis, OR
- TP 117 **Exploring Proteomic Signatures Linked to Early Life Exposure in Atopic Dermatitis and Asthma : ECHO-COCOA Study;** Seungyoon Seo<sup>1</sup>; Yeonwoo Jo<sup>1</sup>; Hwangkyo Jeong<sup>1</sup>; Hosub Im<sup>2</sup>; Mi-Jin Kang<sup>3</sup>; Soo-Jong Hong<sup>4</sup>; Jeonghun Yeom<sup>1</sup>; <sup>1</sup>Prometabio Research Institute, prometabio co., Ltd., Hanam-si, South Korea; <sup>2</sup>Institute for Life & Environmental Technology, Smarteye Corporation, Hanam-si, South Korea; <sup>3</sup>Humidifier Disinfectant Health Center, Asan Medical Center, Songpa-gu, South Korea; <sup>4</sup>Department of Pediatrics, Childhood Asthma Atopy Center, Humidifier Disinfectant Health Center, Asan Medical Center, University of Ulsan College of Medicine, Songpa-gu, South Korea

### FOOD SAFETY & CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS, AND SUPPLEMENTS II 118-137

- TP 118 **Determination of Limonin in Citrus Flour by Time of Flight (TOF) LC/MS;** Sue D'Antonio<sup>1</sup>; Donna Payne<sup>2</sup>; John Wright<sup>3</sup>; Michael Adams<sup>4</sup>; <sup>1</sup>Agilent Technologies Inc., Cedar Creek, TX; <sup>2</sup>AnalytEval, SMITHVILLE, TX; <sup>3</sup>Agilent Technologies, Wilmington, DE; <sup>4</sup>CWC Labs, Cedar Creek, TX
- TP 119 **Overcoming Sampling Challenges in Analyzing Retained Tea Flavor Using Soft Ionization by Chemical Reaction in Transfer (SICRIT);** Xinwei Feng<sup>1</sup>; Hui Li<sup>1</sup>; Ying Xu<sup>1</sup>; <sup>1</sup>The Coca-Cola Company, Shanghai, China
- TP 120 **Continued Method Development of a Quantitative Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) Method for Analyzing Diarrhetic Shellfish Toxins;** Christopher R. Beekman<sup>1</sup>; Brigid Carr<sup>2</sup>; Daniel Chavez<sup>3</sup>; Shelley K. Lankford<sup>3</sup>; Stephen D. Archer<sup>2</sup>; Jonathan R. Deeds<sup>1</sup>; <sup>1</sup>U.S. Food and Drug Administration, College Park, MD; <sup>2</sup>Bigelow Laboratory for Ocean Sciences, East Boothbay, ME; <sup>3</sup>Washington State Department of Health Public Health Laboratories, Shoreline, WA
- TP 121 **Proteomics for species authentication of cod and corresponding fishery products;** Han-ju Chien<sup>1</sup>; Yu-Han Huang<sup>2</sup>; Yi-Feng Zheng<sup>3</sup>; Wei-Chen Wang<sup>3</sup>; Cheng-Yu Kuo<sup>3</sup>; Guor-Jien Wei<sup>2,4</sup>; Chien-Chen Lai<sup>3,5,6</sup>; <sup>1</sup>Department of Biochemical Science and Technology, National Chiayi University, Chiayi city, Taiwan; <sup>2</sup>Institute of Food Safety and Health Risk Assessment, National Yang-Ming University, Taipei city, Taiwan; <sup>3</sup>Institute of Molecular Biology, National Chung Hsing University, Taichung city, Taiwan; <sup>4</sup>Metabolomics-Proteomics Research Center, National Yang-Ming University, Taipei city, Taiwan; <sup>5</sup>Advanced Plant Biotechnology Center, National Chung Hsing University, Taichung city, Taiwan; <sup>6</sup>Graduate Institute of Chinese Medical Science, China Medical University, Taichung city, Taiwan
- TP 122 **Multitomic Analysis for Identifying Adulteration, Geographical Origins, and Species in Soy Sauce;** Wei-chen Wang<sup>1</sup>; Shau-Chun Wang<sup>2</sup>; Chien-Chen Lai<sup>3,4,5,6</sup>;

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- <sup>1</sup>National Chung Hsing University, Taichung, Taiwan; <sup>2</sup>National Chung Cheng University, Chiayi city, Taiwan; <sup>3</sup>Institute of Molecular Biology, National Chung Hsing University, Taichung, Taiwan; <sup>4</sup>Advanced Plant Biotechnology Center, National Chung Hsing University, Taichung city, Taiwan; <sup>5</sup>Ph.D. Program in Translational Medicine, National Chung Hsing University, Taichung, Taiwan; <sup>6</sup>Rong Hsing Research Center for Translational Medicine, National Chung Hsing University, Taichung, Taiwan
- TP 123 **Analyzing Nitrosamines with Hydrogen Carrier Gas: GC/MS/MS Analysis of Nitrosamines in Sartan Drugs;** Soma Dasgupta<sup>1</sup>; Parul Angrish<sup>2</sup>; Anastasia Andrianova<sup>3</sup>; Joel Ferrer<sup>2</sup>; <sup>1</sup>Agilent technologies, Bangalore, India; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>Agilent Technologies, Wilmington, DE
- TP 124 **Development of a generic fish MS detection method for allergen control;** Justin Marsh<sup>1</sup>; Tengfei Li<sup>1</sup>; Joseph Baumert<sup>1</sup>; Philip Johnson<sup>1</sup>; <sup>1</sup>University of Nebraska - Lincoln, Lincoln, NE
- TP 125 **Identification of covalent protein-flavonoid interactions using intact and bottom-up mass spectrometry;** P. Matthew Joyner<sup>1</sup>; Abigail Martinez Valdovinos<sup>1</sup>; Alyssa Hornback<sup>1</sup>; <sup>1</sup>Pepperdine University, Malibu, CA
- TP 126 **Novel Analytical Approach to The Quantitation of Bovine Immunoglobulin G Using Isoform-Specific Peptide Markers and Liquid Chromatography – Mass Spectrometry;** Stefan Ehling<sup>1</sup>; Matthew K Fleshman<sup>1</sup>; <sup>1</sup>Abbott Nutrition, Columbus, OH
- TP 127 **Exploring the Impact of Protein Digestibility on Food Allergenicity through DIA-MS Profiling;** Chee Fan TAN<sup>1</sup>; Ai Che YAP<sup>2</sup>; Felicia Yu Yin ONG<sup>1</sup>; Hui Ru TAN<sup>3</sup>; Yao Xing WONG<sup>3</sup>; Weibiao ZHOU<sup>2</sup>; Juan DU<sup>3</sup>; Xuezhi Bi<sup>1, 3</sup>; <sup>1</sup>Bioprocessing Technology Institute, Agency for Science, Technology and Research, Singapore, Singapore; <sup>2</sup>Department of Food Science and Technology, National University of Singapore, Singapore, Singapore; <sup>3</sup>Food, Chemical and Biotechnology Cluster, Singapore Institute of Technology, Singapore, Singapore
- TP 128 **Calibrant extraction and digestion for the development of an MS gluten detection method in fermented and hydrolyzed foods;** Sara K Schlange<sup>1</sup>; Joseph L Baumert<sup>1</sup>; Melanie L Downs<sup>1</sup>; <sup>1</sup>University of Nebraska-Lincoln, Lincoln, NE
- TP 129 **Combining Proteomics and Metabolomics to Assess Food Protein Digestibility;** Cheng-Yu Weng<sup>1</sup>; Shawn Ehlers-Cheang<sup>1</sup>; Nikita Bacalzo<sup>1</sup>; Emelie Strandberg<sup>2</sup>; Fangzhou Li<sup>3</sup>; Mariana Barboza<sup>4</sup>; Justin B. Siegel<sup>1</sup>; Ilias Tagkopoulos<sup>3</sup>; Keith Baar<sup>2</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of California, Davis, Davis, CA; <sup>2</sup>College of Biological Sciences, University of California, Davis, Davis, CA; <sup>3</sup>Department of Computer Science, University of California, Davis, Davis, CA; <sup>4</sup>Innovation Institute for Food and Health, University of California, Davis, Davis, CA
- TP 130 **Discrimination of foodborne pathogens associated with outbreaks using Tandem Liquid Chromatography Ion Mobility Mass Spectrometry (LC-IM-MS/MS);** Jessica S. Pizzo<sup>1</sup>; Sheba P. Maaji<sup>1</sup>; Iffat Jerin<sup>1</sup>; Kimberly Y. Kartowikromo<sup>1</sup>; Orobola E. Olajide<sup>1</sup>; Ahmed M. Hamid<sup>1</sup>; <sup>1</sup>Auburn University, AUBURN, AL
- TP 131 **Non-targeted metabolomics analysis for structural elucidation of tannins using high-resolution mass spectrometry;** HONG-JHANG CHEN<sup>1</sup>; GUI-RU XIE<sup>1</sup>; <sup>1</sup>Institute of Food Science and Technology, National Taiwan University, Taipei, Taiwan
- TP 132 **Prevention of age-related diseases by taking Black chokeberry;** Takuva Yamane<sup>1, 2</sup>; Yu Nakajima<sup>1</sup>; Momoko Imai<sup>1, 2</sup>; Takeshi Bamba<sup>2, 3</sup>; Susumu Uchiyama<sup>1, 2</sup>; <sup>1</sup>Osaka University, Suita, Japan; <sup>2</sup>BYU-Analytica Inc., Osaka, Japan; <sup>3</sup>Kyushu university, Fukuoka, Japan
- TP 133 **Chemical profiling and quantification of major royal jelly protein of royal jelly products using non-targeted and targeted metabolomics;** HONG-JHANG CHEN<sup>1</sup>; CHUN-CHIEH CHANG<sup>2</sup>; GUI-RU XIE<sup>1</sup>; <sup>1</sup>Institute of Food Science and Technology, National Taiwan University, Taipei, Taiwan; <sup>2</sup>Hsinlin Biomedical Co., Ltd., Yilan, Taiwan
- TP 134 **Analysis of Pharmacokinetics of Whole Coffee Fruit Caffeine Extract in Human Serum by Liquid Chromatography Mass Spectrometry;** Nebiyu Abshiru<sup>1</sup>; Zb Pietrkowski<sup>2</sup>; Boris Nemzer<sup>2, 3</sup>; <sup>1</sup>FutureCeuticals, Momence, IL; <sup>2</sup>VDF FutureCeuticals, Inc., Momence, IL; <sup>3</sup>University of Illinois at Urbana-Champaign, Urbana, IL
- TP 135 **The Elemental Palette: Ionomic profiling across 500 diverse food samples;** Jacqueline Michelle Chaparro<sup>1</sup>; Rachel R Jones<sup>1</sup>; John C Evans<sup>1</sup>; Macy Gruszczynski<sup>1</sup>; Margaret Read<sup>1</sup>; Susan B Mitchell<sup>1</sup>; Melanie T Odenkirk<sup>1</sup>; Corey D Broeckling<sup>1</sup>; Tracy Shafizadeh<sup>2</sup>; Steven Watkins<sup>2</sup>; Jessica E Prenni<sup>1</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO; <sup>2</sup>Verso Biosciences, Davis, CA
- TP 136 **Determination of 87 veterinary drug, pesticide and mycotoxin residues in beef by ionic liquid-dispersive liquid-liquid microextraction/liquid chromatography-mass spectrometry;** Sandy SO Mookantsa<sup>1, 2</sup>; Simiso Dube<sup>1</sup>; Mathew MM Nindi<sup>1</sup>; <sup>1</sup>University of South Africa, Florida Park, Roodepoort, South Africa; <sup>2</sup>Botswana National Veterinary Laboratory, Gaborone, Botswana
- TP 137 **Comparison of protein changes in donor human milk after Holder pasteurization, high-pressure process and UV-C treatment;** Bum Jin Kim<sup>1</sup>; Hussein M.H. Mohamed<sup>1</sup>; Austin Lowder<sup>2</sup>; Joy Waite-Cusic<sup>1</sup>; David Dallas<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR; <sup>2</sup>JBT Corporation, Erlanger, KY
- FUNDAMENTALS: ION MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS**  
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- TP 138 **The Energy Dependence of Transuranic Cation Reactions with Methane Observed by ICP-MS/MS;** Richard Cox<sup>1</sup>; Amanda D. French<sup>1</sup>; Kali M. Melby<sup>1</sup>; Michael J. Rodriguez<sup>1</sup>; Wenjin Cao<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- TP 139 **Comparison of solution and gas phase structural ensembles of denatured cytochrome c;** Rebecca L Cain<sup>1</sup>; Ian K Webb<sup>1</sup>; <sup>1</sup>Indiana University Purdue University Indianapolis, Indianapolis, IN
- TP 140 **Complexation of Phosphate Groups with Diserinol Isophthalamide in Electrospray Ionization Mass Spectrometry;** Neil A Ellis<sup>1</sup>; Madeline Schultz<sup>1</sup>; Daniel A Thomas<sup>1</sup>; <sup>1</sup>University of Rhode Island, Kingston, RI
- TP 141 **Developing various length gaseous electrostatic to covalent crosslinkers: towards understanding the effects of solvation and desolvation on protein structure;** Kacy L Black<sup>1</sup>; Ian K. Webb<sup>1</sup>; <sup>1</sup>IUPUI, Indianapolis, IN
- TP 142 **Diagnostic Gas-Phase Ion-Molecule Reactions of Tris(dimethylamino)borane Coupled with Collision-Associated Dissociation for the Mass Spectrometric Identification of Secondary Hydroxylamines;** Annika M Little<sup>1</sup>; Hilka I Kenttämää<sup>1</sup>; Keriany Fuentes<sup>2</sup>; Charles M Pletcher<sup>1</sup>; Jack C Howard<sup>1</sup>; Daria T Tsoneva<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>University of Puerto Rico Humacao, Humacao, Puerto Rico
- TP 143 **Probing Metal Ion Adduction in the Charged Residue Mechanism of ESI via Gas-Phase Ion-ion Chemistry;** Alexander M. Koers<sup>1</sup>; Nicole M. Brundridge<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- TP 144 **Protecting ETD Singly-charged Products from Further Reaction via Enhanced Singly-charged Scans;** Seth A. Horn<sup>1</sup>; Kimberly C. Fabijanczuk<sup>1</sup>; Ian J. Carrick<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University Department of Chemistry, West Lafayette, IN
- TP 145 **Nitrosation of the One-Electron Oxidized Guanine and 9-Methylguanine by Nitric Oxide;** Jonathan Benny<sup>1, 2</sup>; Jianbo

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- TP 146 **Li<sup>1,2</sup>; <sup>1</sup>The Graduate Center of the City University of New York, New York, NY; <sup>2</sup>Queens College CUNY, Flushing, NY Investigation into the Reaction Dynamics of Guanine-Amine Cross-links Mediated by One- and Two-Electron Oxidation Using Electrospray Ionization Tandem Mass Spectrometry; May Myat Moe<sup>1,2</sup>; Jonathan Benny<sup>1,2</sup>; Jianbo Liu<sup>1,2</sup>; <sup>1</sup>Queens College CUNY, Flushing, NY; <sup>2</sup>The Graduate Center of the City University of New York, New York, NY**
- TP 147 **Ion Parking in a Home-Built Digital 3D Quadrupole Ion Trap: Expected Challenges and Relevant Calculations; Liangxuan Fu<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University Department of Chemistry, West Lafayette, IN**
- TP 148 **Understanding ligand-exchange of Ni and Fe complexes on surfaces using ion soft-landing; Raquel Cericatto Konzen<sup>1</sup>; Hugo Y. Samayoa-Oviedo<sup>1</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN**
- TP 149 **Origin of the unexpected Rb<sup>+</sup> (or K<sup>+</sup>) detection from collisional activation of sodiated cyclodepsipeptides; Chengqin Cao<sup>1</sup>; Sophie Liuu<sup>2</sup>; Ekaterina Darii<sup>3</sup>; Yves Gimbert<sup>4</sup>; Annelaure DAMONT<sup>1</sup>; Olivier Firmesse<sup>2</sup>; François FENAILLE<sup>1</sup>; Jean-Claude Tabet<sup>1,4</sup>; <sup>1</sup>Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), MetaboHUB, Gif-sur-Yvette, France; <sup>2</sup>Staphylococcus, Bacillus and Clostridium unit (SBCL), Laboratory for Food Safety, French Agency for Food, Environmental and Occupational Health & Safety (ANSES), Université Paris-Est, Maisons-Alfort, France; <sup>3</sup>Génomique métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry, France.; Evry, France; <sup>4</sup>Faculté des Sciences et de l'Ingénierie, Institut Parisien de Chimie Moléculaire (IPCMI), Sorbonne Université, Paris, France**
- TP 150 **Top-down characterization of intact proteins via on-line charge-stripping and electron capture dissociation; Yury V. Vasilev<sup>1</sup>; Michael C. Hare<sup>1</sup>; Ruwan T. Kurulugama<sup>2</sup>; Joseph C. Meeuwssen<sup>1</sup>; Bill Russ<sup>2</sup>; <sup>1</sup>Agilent Technologies, CORVALLIS, OR; <sup>2</sup>Agilent Technologies, Santa Clara, CA**
- TP 151 **Comparison of Gas Phase Fragmentation Behaviors of Nuclear Fuel Cycle Ligands in Lanthanide and Americium Metal Ligand; JungSoo Kim<sup>1</sup>; Christopher A. Zarzana<sup>1</sup>; Brittany D. M. Hodges<sup>1</sup>; Corey D. Pilgrim<sup>1</sup>; <sup>1</sup>Idaho National Laboratory, Idaho Falls, ID**
- TP 152 **Electron Energy vs Density Effects in Peptide Cation-Electron Reactions: Proposed Alternative Fragmentation Mechanisms and Unexpected Observations; Steven A. DeFiglia<sup>1</sup>; Neven N. Mikawy<sup>1</sup>; Teresa Lee<sup>1</sup>; Kristina Håkansson<sup>1</sup>; <sup>1</sup>University of Michigan Department of Chemistry, Ann Arbor, MI**
- TP 153 **Preliminary Implementation of a Xenon Reagent for Negative Electron Transfer Dissociation on Orbitrap Tribrid™ Systems; Keaton L Mertz<sup>1</sup>; Daniel J Nesbitt<sup>1</sup>; Joshua J Coon<sup>1,2,3,4</sup>; <sup>1</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>Morgridge Institute for Research, Madison, WI; <sup>4</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI**
- TP 154 **Ion Mobility Separation by means of Space Charge in Accumulation Regions with high concentrations; Amirreza Tootchi<sup>1</sup>; Viraj D Gandhi<sup>1,2</sup>; Farah Mubas-Sirah<sup>1</sup>; Carlos Larriba-Andaluz<sup>1</sup>; <sup>1</sup>Indiana University Purdue University Indianapolis, Indianapolis, IN; <sup>2</sup>Purdue University, West Lafayette, IN**
- TP 155 **Native LC-MS Method Development for Characterization of Biologics on Orbitrap Eclipse Coupled with Acquity Premier UPLC; Zhihao Yu<sup>1</sup>; Jacob Furlon<sup>1</sup>; Zhili Li<sup>1</sup>; <sup>1</sup>Insmad, Bridgewater, NJ**
- TP 156 **Native Top-Down Mass Spectrometry for Characterizing Sarcomeric Proteins Directly from Cardiac Tissue Lysate; Brad Li<sup>1</sup>; Emily A Chapman<sup>2</sup>; Kevin M Buck<sup>2</sup>; Hsin-Ju Chan<sup>2</sup>; Boris Krichel<sup>2</sup>; David S Roberts<sup>2</sup>; Ying Ge<sup>2,3,4</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Biochemistry, Madison, WI; <sup>2</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, WI; <sup>3</sup>University of Wisconsin-Madison, Department of Cell and Regenerative Biology, Madison, WI; <sup>4</sup>Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI**
- TP 157 **Measuring Effects of Biochemically Relevant Salts on Protein Stability and Conformation using Native Mass Spectrometry; Katherine J Lee<sup>1</sup>; Jacob S Jordan<sup>1</sup>; Evan R Williams<sup>1</sup>; <sup>1</sup>University of California, Berkeley, Berkeley, CA**
- TP 158 **Affinity Painting of Membrane Protein-Lipid Interactions with Native Mass Spectrometry; Farhana Afrin Mohona<sup>1</sup>; Hiruni S. Jayasekera<sup>1</sup>; Megan Ewbank<sup>1</sup>; Michael Marty<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ**
- TP 159 **Direct Analysis of SEC Fractionated E. coli Protein Complexes using Matrix-Landing Mass Spectrometry; Noah M Lancaster<sup>1,2</sup>; Austin Z Salome<sup>1,2</sup>; Drew Jordahl<sup>2</sup>; Colin Hemme<sup>3,4</sup>; Keaton L Mertz<sup>1</sup>; Mitchell D Probasco<sup>4</sup>; Erin L Metter<sup>2</sup>; Patricia J Kiley<sup>2</sup>; Michael S Westphall<sup>2,5</sup>; Scott T Quarmby<sup>2,5</sup>; Timothy Grant<sup>3,4</sup>; Joshua J Coon<sup>1,2,4,5</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, WI; <sup>2</sup>University of Wisconsin-Madison, Department of Biomolecular Chemistry, Madison, WI; <sup>3</sup>University of Wisconsin-Madison, Department of Biochemistry, Madison, WI; <sup>4</sup>Morgridge Institute for Research, Madison, WI; <sup>5</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI**
- TP 160 **Exploring cryo-electron microscopy compatible matrices for room temperature soft landing of macromolecules; Drew Jordahl<sup>1</sup>; Austin Z Salome<sup>1,2</sup>; Colin Hemme<sup>3,4</sup>; Keaton L Mertz<sup>1,2</sup>; Mitchell D Probasco<sup>4</sup>; Michael S Westphall<sup>1,5</sup>; Scott T Quarmby<sup>1,5</sup>; Timothy Grant<sup>3,4</sup>; Joshua J Coon<sup>1,2,4,5</sup>; <sup>1</sup>Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>Department of Biochemistry, University of Wisconsin-Madison, Madison, WI; <sup>4</sup>Morgridge Institute for Research, Madison, WI; <sup>5</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI**
- TP 161 **Monitoring Effects of Nonvolatile Buffers on Assembly of Protein Complexes Using Native Mass Spectrometry and Ultraviolet Photodissociation; Hanlin Ren<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Texas at Austin, Austin, TX**
- TP 162 **Modeling the efficiency of collisional energy transfer and activation for native protein ions; Austin W Green<sup>1</sup>; Samantha Shepherd<sup>1</sup>; Ruwan Kurulugama<sup>2</sup>; Kenneth Newton<sup>1</sup>; James Prell<sup>1</sup>; <sup>1</sup>University of Oregon, Eugene, OR; <sup>2</sup>Agilent Technologies, Santa Clara, CA**
- TP 163 **Direct Measurement of Binding Affinities of Weak Protein-Protein Interactions via Submicron Emitters and Native Mass Spectrometry; Chae Kyung Jeon<sup>1</sup>; Emily G Sweeney<sup>1</sup>; Michael J Harms<sup>1</sup>; Karen Guillemin<sup>1</sup>; James S Prell<sup>1</sup>; <sup>1</sup>University of Oregon, Eugene, OR**
- TP 164 **Mechanistic insights into slow mixing in SLOMO-nMS; Simar K. Dhillon<sup>1</sup>; Duong T. Bui<sup>1</sup>; Elena N. Kitova<sup>1</sup>; Lara K. Mahal<sup>1</sup>; Morris R. Flynn<sup>1</sup>; John S. Klassen<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, AB**
- TP 165 **Elusive Protein-Glycosphingolipid Interactions Revealed by Membrane Anchor-Assisted (MEAN) Native Mass Spectrometry; James W. Favell<sup>1</sup>; Duong T. Bui<sup>1</sup>; Jianing Li<sup>1</sup>; Ling Han<sup>1</sup>; Elena N. Kitova<sup>1</sup>; Edward N. Schmidt<sup>1</sup>; Pavel I. Kitov<sup>1</sup>; Lara K. Mahal<sup>1</sup>; Yves St-Pierre<sup>2</sup>; Matthew S. Macauley<sup>1,3</sup>; John S. Klassen<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Alberta, Edmonton, AB; <sup>2</sup>INRS-Institut Armand-Frappier, Laval, QC; <sup>3</sup>Department of Medical Microbiology and Immunology, University of Alberta, Edmonton, AB**
- TP 166 **A Multidimensional Native Separation for the Online Analysis of Endogenous Protein Complexes from Human Heart Tissue; Matthew S Fischer<sup>1</sup>; Holden T**

### FUNDAMENTALS: NATIVE MS 155-171

## TUESDAY POSTERS

- Rogers<sup>1</sup>; Emily A Chapman<sup>2</sup>; Boris Krichel<sup>3, 4</sup>; Eli J Larson<sup>2</sup>; Zhan Gao<sup>3</sup>; Andrew J Alpert<sup>5</sup>; Ying Ge<sup>2, 3, 6</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, WI; <sup>2</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin; <sup>3</sup>University of Wisconsin-Madison, Department of Cell and Regenerative Biology, Madison, WI; <sup>4</sup>School of Life Sciences, University of Siegen, Siegen, Germany; <sup>5</sup>PolyLC Inc, Columbia, MD; <sup>6</sup>Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI
- TP 167 **Mapping protein structure stability for native mass spectrometry with vibrating sharp-edge spray ionization.**; Mst Nigar Sultana<sup>1</sup>; Vikum Dewasurendra<sup>2</sup>; Matthew Johnson<sup>1</sup>; Sultan Mahmud<sup>3</sup>; Mohammad Rahman<sup>3</sup>; Stephen Valentine<sup>3</sup>; Peng Li<sup>3</sup>; <sup>1</sup>West Virginia University, Morgantown, WV; <sup>2</sup>West Virginia University, Morgantown, WV; <sup>3</sup>West Virginia University- C. Eugene Bennett Department of Chemistry, Morgantown, WV
- TP 168 **Native and native top-down mass spectrometry analysis of endogenous membrane proteins and their bound ligands directly from membranes;** Wonhyeuk Jung<sup>1</sup>; Aniruddha Panda<sup>2</sup>; Kallol Gupta<sup>2</sup>; <sup>1</sup>Yale University, New Haven, CT; <sup>2</sup>Yale University, West Haven, CT
- TP 169 **On the “Freeze-Drying” [1] of Protein Solution Structures in the Absence of Solvent: Rugged Energy Landscape and Glass-Like Behavior;** Christian Bleiholder<sup>1</sup>; Tyler C. C Cropley<sup>1</sup>; Fanny C Liu<sup>1</sup>; Mengqi Chai<sup>2</sup>; Thais Pedrete<sup>1</sup>; Jusung Lee<sup>1</sup>; <sup>1</sup>Florida State University, Tallahassee, FL; <sup>2</sup>Washington University in Saint Louis, St. Louis, MO
- TP 170 **Deep Ultraviolet and Infrared Laser Ablation of Carbonic Anhydrase II;** Neda Feizi<sup>1</sup>; Kadeem O Hayes<sup>2</sup>; Blessing Chisom Egbejiogu<sup>2</sup>; Kelcey B. Hines<sup>2</sup>; Kermit K. Murray<sup>2</sup>; Touradj Solouki<sup>1</sup>; <sup>1</sup>Baylor University, Waco, TX; <sup>2</sup>Louisiana State University, Baton Rouge, LA
- TP 171 **Cryogenic Soft Landing Improves Structural Preservation of Protein Complexes;** Austin Z Salome<sup>1, 2</sup>; Kenneth W Lee<sup>2</sup>; Colin Hemme<sup>3, 4</sup>; Michael S Westphall<sup>2, 5</sup>; Keaton L Mertz<sup>1, 2</sup>; Mitchell D Probasco<sup>4</sup>; Scott T Quarmby<sup>2, 5</sup>; Timothy Grant<sup>3, 4</sup>; Joshua J Coon<sup>1, 2, 4, 5</sup>; <sup>1</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>Department of Biochemistry, University of Wisconsin-Madison, Madison, WI; <sup>4</sup>Morgridge Institute for Research, Madison, WI; <sup>5</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI
- HIGH THROUGHPUT MS I**  
 172-196
- TP 172 **Determination of binding affinity with Rapid Equilibrium Dialysis (RED) and LC-MS;** Bryan Choi<sup>1</sup>; Calvin Han<sup>1</sup>; Jonathan LaRochelle<sup>1</sup>; Damian Houde<sup>1</sup>; <sup>1</sup>Relay Therapeutics, Cambridge, MA
- TP 173 **Nano-ASMS: Nanoscale Synthesis and Affinity Ranking with Acoustic Ejection Mass Spectrometry and Affinity Selection Mass Spectrometry;** Jerry Barney; Bristol Myers Squibb, Princeton, NJ
- TP 174 **High-throughput MS-based cholesterol quantitation assay for Niemann-Pick Disease type C (NPC);** Yuhong Fang<sup>1</sup>; Yi-Han Lin<sup>1</sup>; Maya L. Gosztyla<sup>1</sup>; Edward Zhu<sup>1</sup>; Abhijeet Kapoor<sup>1</sup>; Andrés E. Dulcey<sup>1</sup>; Daniel C. Talley<sup>1</sup>; Mark J. Henderson<sup>1</sup>; Xin Hu<sup>1</sup>; Wei Zheng<sup>1</sup>; Anton Simeonov<sup>1</sup>; Juan J. Marugan<sup>1</sup>; Christopher A LeClair<sup>1</sup>; Bolormaa Baljinnyam<sup>1</sup>; Dingyin Tao<sup>1</sup>; <sup>1</sup>National Center for Advancing Translational Sciences, NIH, Rockville, MD
- TP 175 **High-throughput Characterization of Therapeutic Proteins by Peptide Mapping Using Ultra-High Pressure Liquid Chromatography Mass Spectrometry;** Andrew B. Dykstra<sup>1</sup>; Prashant N. Jethva<sup>1</sup>; Daniel W. Woodall<sup>1</sup>; Pavel V. Bondarenko<sup>1</sup>; <sup>1</sup>Amgen, Thousand Oaks, CA
- TP 176 **High-throughput Mass Spectrometry - Based Detec--tion of Deamination Activity of ADAR1 without Prior Separation;** Yating Wang<sup>1</sup>; Travis Pemberton<sup>1</sup>; Ping Zhang<sup>2</sup>; Iyoncey Rodrigo<sup>2</sup>; Zhigang Wang<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb, Cambridge, MA; <sup>2</sup>Bristol Myers Squibb, Lawrenceville, NJ
- TP 177 **Pushing the limits of uncompromised high-throughput HCP profiling with utmost speed and sensitivity;** Kristina Srzentic<sup>1</sup>; Kai Scheffler<sup>2</sup>; Florian Bonn<sup>3</sup>; Tabiwang Arrey<sup>3</sup>; Nicolae Eugen Damoc<sup>3</sup>; Ales Holfeld<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Reinach, Switzerland; <sup>2</sup>Thermo Fisher Scientific, Germering, Germany; <sup>3</sup>Thermo Fisher Scientific, Bremen, Germany
- TP 178 **Rapid determination of four anions in urine;** Xiao Luo<sup>1</sup>; Yanjian Wan<sup>2</sup>; Liuting Zhao<sup>3</sup>; Zong Yang<sup>3</sup>; Bingjie Liu<sup>3</sup>; Lihai Guo<sup>3</sup>; <sup>1</sup>Key Laboratory of Environment and Health, Tongji Medical College, Huazhong University of Science and Technology, Wuhan, China; <sup>2</sup>Center for Public Health Laboratory Service, Institute of Environmental Health, Wuhan Centers for Disease Control & Prevention, Wuhan, China; <sup>3</sup>SCIEX Asia Pacific Application Support Center,, Shanghai, China
- TP 179 **OPSI-MS: System integration for high-throughput bioanalysis;** Manan Luthra<sup>1</sup>; Savannah Wood<sup>1</sup>; Nate Hoxie<sup>1</sup>; Vijay Veerisetty<sup>1</sup>; Anthony Garrison<sup>1</sup>; Pranav Bende<sup>1</sup>; John Janiszewski<sup>1</sup>; Jonathan Shrimp<sup>1</sup>; Meghav Verma<sup>1</sup>; Sam Michael<sup>1</sup>; Matthew D Hall<sup>1</sup>; Peter Kovarik<sup>2</sup>; Tom Covey<sup>2</sup>; Chang Liu<sup>2</sup>; <sup>1</sup>NIH/NCATS, Rockville, Maryland; <sup>2</sup>SCIEX, Concord, ON
- TP 180 **High-throughput affinity selection-mass spectrometry system using novel nanoparticle ferrimagnetic beads;** Richard B. Van Breemen<sup>1</sup>; Jenna Miller<sup>2</sup>; Nate Hoxie<sup>2</sup>; Meghav Verma<sup>2</sup>; Michael Ronzetti<sup>2</sup>; John Janiszewski<sup>2</sup>; Bolormaa Baljinnyam<sup>2</sup>; Jonathan Shrimp<sup>2</sup>; Anton Simeonov<sup>2</sup>; Sam Michael<sup>2</sup>; Matthew D Hall<sup>2</sup>; Daniel Simchuk<sup>1</sup>; Jianli Zhao<sup>3</sup>; Sasikumar Pillai<sup>4</sup>; Babu Purkayastha<sup>4</sup>; Peter Kovarik<sup>5</sup>; Tom Covey<sup>5</sup>; Chang Liu<sup>5</sup>; <sup>1</sup>Oregon State University, Corvallis, OR; <sup>2</sup>National Center for Advancing Translational Sciences (NCATS), Rockville, MD; <sup>3</sup>Phenomenex, Torrance, CA; <sup>4</sup>Sciex, Framingham, MA; <sup>5</sup>SCIEX, Concord, ON
- TP 181 **Automatic cleaning in Acoustic Ejection Mass Spectrometry: Enhancing the system robustness for large-scale high-throughput analysis of complex samples;** Huguang Ji<sup>1</sup>; Xuejiao Yin<sup>1</sup>; Wan Ee Ang<sup>1</sup>; Abdullah Bin Rawshan<sup>1</sup>; Susan Gay<sup>1</sup>; Jing Ma<sup>1</sup>; Chiu Cheong Aw<sup>1</sup>; Parikshit Gokhale<sup>2</sup>; Chang Liu<sup>2</sup>; <sup>1</sup>SCIEX, Singapore, Singapore; <sup>2</sup>SCIEX, Concord, ON
- TP 182 **Development of high throughput isotope dilution protocols for I.DOT/OPSI-MS for determination of nitrification and mineralization rates in soil;** John F. Cahill<sup>1</sup>; Vilmos Kertesz<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN
- TP 183 **A faster scanning DIA approach for high throughput quantitative proteomics;** Anjali Chelur<sup>1</sup>; Stephen Tate<sup>1</sup>; Claudia Alvarez<sup>1</sup>; Gordana Ivosev<sup>1</sup>; Nic G Bloomfield<sup>1</sup>; <sup>1</sup>SCIEX, Concord, ON
- TP 184 **Optimisation of DIA-PASEF permits retrospective, high throughput proteomics of trizol-extracted biopsies from Metabolic dysfunction associated steatotic liver disease (MASLD) patients;** Andrew M Frey<sup>1</sup>; Andrew Porter<sup>1</sup>; Pawel Palmowski<sup>1</sup>; Quentin M Anstee<sup>1</sup>; Ann Daly<sup>1</sup>; Matthias Trost<sup>1</sup>; <sup>1</sup>Newcastle University, Newcastle upon Tyne, United Kingdom
- TP 185 **A complete and automated end-to-end sample preparation strategy for high-throughput and standardized proteomics with high sensitivity;** Magnus Huusfeldt<sup>1</sup>; Hope Cabalo Zisco<sup>1</sup>; Dorte B Bekker-Jensen<sup>1</sup>; Nicolai H Bache<sup>1</sup>; <sup>1</sup>Evosep, Odense, Denmark
- TP 186 **Inter-laboratory assessment of standardized and fully automated, sample preparation workflows integrated with EvosepOne;** Andrea Ellero<sup>1, 2</sup>; Camilla O. Kuhl<sup>3</sup>; Joel M. Vej-Nielsen<sup>3</sup>; Adele Nel<sup>1, 2</sup>; Anne Katrine Ravno<sup>3</sup>; Ireshyn S Govender<sup>1, 4</sup>; Previn Niacker<sup>1, 4</sup>; Stoyan Stoychev<sup>3, 5</sup>; Dorte B. Bekker-Jensen<sup>3</sup>; Nicolai Bache<sup>3</sup>; Justin Jordaan<sup>1</sup>; <sup>1</sup>ReSyn Biosciences, Pretoria, South Africa; <sup>2</sup>University of Pretoria,

## TUESDAY POSTERS

- Pretoria, South Africa; <sup>3</sup>Veosep, Odense, Denmark; <sup>4</sup>Council for Scientific and Industrial research, Pretoria, South Africa; <sup>5</sup>ReSyn BioSciences, Johannesburg, South Africa
- TP 187 **Next-generation Acoustic Ejection Mass Spectrometry: A fully automated platform for high-throughput sample analysis;** Jacob Watson McCabe<sup>1</sup>; Aaron Stella<sup>1</sup>; Anuja Bhalkikar<sup>1</sup>; Heidi D Paolieri<sup>2</sup>; Marisa A Spence<sup>2</sup>; Sarah Simons<sup>2</sup>; Han Joo Lee<sup>1</sup>; <sup>1</sup>SCIEX, USA, Framingham, MASSACHUSETTS; <sup>2</sup>Beckman Coulter Life Sciences, Indianapolis, IN
- TP 188 **A high-throughput, compound agnostic target engagement assay for covalent inhibitors of G12C KRAS using acoustic droplet ejection mass spectrometry;** Michelle Robinson<sup>1</sup>; Rajesh Desai<sup>1</sup>; Nicolas Solban<sup>2</sup>; Weixun Wang<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., West Point, PA; <sup>2</sup>Merck, Boston, MA
- TP 189 **Affinity-Selection Mass Spectrometry (MagMASS) for the Discovery of Ligands for the SHIP1 protein involved in Alzheimer's Disease;** Daniel D Simchuk<sup>1, 2</sup>; Andrew D Mesecar<sup>3</sup>; Adam K Hamdani<sup>3</sup>; Richard Van Breemen<sup>1, 2</sup>; <sup>1</sup>Oregon State University, Corvallis, OR; <sup>2</sup>Linus Pauling Institute, Oregon State University, Corvallis, OR; <sup>3</sup>Department of Biochemistry, Purdue University, West Lafayette, IN
- TP 190 **An affinity selection-mass spectrometry screen (ASMS) for identifying novel tyrosine kinase 2 (TYK2) allosteric inhibitors;** Reza Nemati Josheghani<sup>1</sup>; Naifu Zhang<sup>1</sup>; Ronghai Cheng<sup>1</sup>; Daniel Tekverk<sup>1</sup>; Howard Jones<sup>1</sup>; Martin Himmelbauer<sup>1</sup>; <sup>1</sup>Biogen, Cambridge, MA
- TP 191 **High-throughput LC-MS quantification of secreted delta-hemolysin toxin from clinical *S. aureus* isolates;** Ioana Clotea<sup>1</sup>; Magdalena Podkowik<sup>2</sup>; Bo Shopsin<sup>2, 3</sup>; Beatrix Ueberheide<sup>1</sup>; <sup>1</sup>Proteomics Laboratory, Division of Advanced Research Technologies, New York University Grossman School of Medicine, New York, NY; <sup>2</sup>Department of Medicine, Division of Infectious Diseases, NYU Grossman School of Medicine, New York, NY; <sup>3</sup>Department of Microbiology, NYU Grossman School of Medicine, New York, NY
- TP 192 **Mass spectrometry-based screening platform for transition metal nanoparticle catalysis;** Tingyuan Yang<sup>1</sup>; Nilotpal Kapuria<sup>2</sup>; Baixu Zhu<sup>3</sup>; Xingchen Ye<sup>2</sup>; Xin Yan<sup>4</sup>; <sup>1</sup>TAMU, College Station, TX; <sup>2</sup>Indiana University Bloomington, Bloomington, IN; <sup>3</sup>Indiana University, Bloomington, IN; <sup>4</sup>Texas A&M University, College Station, TX
- TP 193 **Ultra-fast Multiplexed LC/MS/MS Using Newly Designed Online SPE Column for the Simultaneous Analysis of Steroid Hormones in Human Serum;** Eishi IMOTO<sup>1</sup>; Vikki JOHNSON<sup>2</sup>; Logan MILLER<sup>1</sup>; Toshiya MATSUBARA<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>2</sup>Shimadzu scientific instruments, Carlsbad, CA
- TP 194 **Development of High-throughput LC-MS/MS Method for UV Stability Study;** Xiaodong Liu; *Corteva Agriscience, Indianapolis, IN*
- TP 195 **High-throughput natural product screening using a multiplexing strategy in combination with a prototype benchtop multi-reflecting time-of-flight mass spectrometer;** Michael J. J. Recchia<sup>1</sup>; Trevor N. Clark<sup>2</sup>; Adam M. King<sup>3</sup>; Lee A Gethings<sup>3</sup>; David Heywood<sup>3</sup>; Roger G. Linington<sup>1</sup>; <sup>1</sup>Simon Fraser University, Burnaby, BC; <sup>2</sup>University of Prince Edward Island, Charlottetown, PEI; <sup>3</sup>Waters Corporation, Wilmslow, United Kingdom
- TP 196 **MetwareBio: Pioneering Mass Spectrometry Innovations for Advanced Metabolomics, Proteomics, and Cloud-Based Research Excellence;** James Dong; *Metware Biotechnology Inc., Woburn*
- TP 198 **Matrix Assisted Laser Desorption Ionisation-Immunohistochemistry (MALDI-IHC) Mass Spectrometry Imaging of Human Tonsil using an Entry-Level Benchtop MALDI-TOF Platform;** Caroline Jones<sup>1</sup>; Simona Salivo<sup>1</sup>; Matthew Openshaw<sup>1</sup>; <sup>1</sup>Kratos Analytical Ltd., Manchester, United Kingdom
- TP 199 **High-Spatial-Resolution Mass Spectrometry Imaging of Phospholipid Biosynthesis-Impaired Mouse Testis via Tapping-Mode Scanning Probe Electro Spray Ionization;** Yoichi Otsuka<sup>1</sup>; Maki Okada<sup>2</sup>; Tomomi Hashidate-Yoshida<sup>3</sup>; Katsuyuki Nagata<sup>3</sup>; Makoto Yamada<sup>4</sup>; Motohito Goto<sup>5</sup>; Mengze Sun<sup>2</sup>; Hideo Shindou<sup>3, 6</sup>; Michisato Toyoda<sup>2</sup>; <sup>1</sup>Osaka University, Toyonaka, Japan; <sup>2</sup>Osaka University, Toyonaka, Japan; <sup>3</sup>National Center for Global Health and Medicine, Shinjuku, Japan; <sup>4</sup>Shimadzu Corporation, Nakagyo-ku, Japan; <sup>5</sup>Central Institute for Experimental Animals, Kawasaki, Japan; <sup>6</sup>The University of Tokyo, Bunkyo-ku, Japan
- TP 200 **Optimisation on the new generation of microscope mode secondary ion mass spectrometry imaging;** Yifeng Jia<sup>1</sup>; Elena Castellani<sup>1, 2</sup>; Felicia Green<sup>2</sup>; Kieran Cheung<sup>3</sup>; Josh Featherstone<sup>3</sup>; Michael Burt<sup>3</sup>; Mark Brouard<sup>3</sup>; Zoltan Takats<sup>2</sup>; <sup>1</sup>Department of Chemistry, University of Oxford, Oxford, United Kingdom; <sup>2</sup>The Rosalind Franklin Institute, Oxford, United Kingdom; <sup>3</sup>Department of Chemistry, University of Oxford, Oxford, United Kingdom
- TP 201 **Characterization of a new MALDI-TOF axial benchtop instrument for MALDI Imaging applications;** Michael Easterling<sup>1</sup>; Sebastian Boehm<sup>2</sup>; Christoph Nordmann<sup>2</sup>; Andreas Haase<sup>2</sup>; Janina Oetjen<sup>2</sup>; Jan Hendrik Kobarg<sup>2</sup>; Tobias Boskamp<sup>2</sup>; Ulrike Schweiger Hufnagel<sup>2</sup>; Jens Christmann<sup>3</sup>; Andrea Tannapfel<sup>3</sup>; Andree Schuster<sup>2</sup>; Katherine Stumpo<sup>1</sup>; Jens Hoehndorf<sup>2</sup>; <sup>1</sup>Bruker Scientific, 40 Manning Road, Billerica, MA; <sup>2</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitsstraße 4, 28359 Bremen, Germany; <sup>3</sup>Institute for Pathology, Ruhr-University Bochum, Bürkle-de-la-Camp-Platz 1, 44789 Bochum, Germany
- TP 202 **An Automated System for High-throughput Nanospray Desorption Electro spray Ionization Mass Spectrometry Imaging;** Lixue Jiang<sup>1</sup>; Emerson Hernly<sup>1</sup>; Benjamin Cerjan<sup>1</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>Purdue University Department of Chemistry, West Lafayette, IN
- TP 203 **Different approaches to 3D Imaging Analysis for observing molecular collision and/or dissociation products;** Joshua Featherstone<sup>1</sup>; Max McCrea<sup>1</sup>; Matt Strutton<sup>1</sup>; Kieran Cheung<sup>1</sup>; Joseph McManus<sup>1</sup>; Chow-shing Lam<sup>1</sup>; Yifeng Jia<sup>1, 2</sup>; Elena Castellani<sup>1, 2</sup>; Felicia Green<sup>2</sup>; Mark Brouard<sup>1</sup>; <sup>1</sup>University of Oxford, Oxford, United Kingdom; <sup>2</sup>Rosalind Franklin Institute, Didcot, United Kingdom
- TP 204 **Improvements in fast mass microscopy for biomedical applications;** Aljoscha Körber<sup>1</sup>; Edith Sandström<sup>1</sup>; Kasper Krijnen<sup>1</sup>; Frans Giskes<sup>1</sup>; Pascal Huysmans<sup>1</sup>; Paul Laeven<sup>1</sup>; Ian G. M. Anthony<sup>1</sup>; Ron M. A. Heeren<sup>1</sup>; <sup>1</sup>Maastricht University, Maastricht, Netherlands
- TP 205 **IR-MALDESI Coupled to a Trapped Ion Mobility Spectrometry and Time-of-Flight Mass Spectrometer;** Kevan T Knizner<sup>1</sup>; Joshua L. Fischer<sup>2</sup>; Mary F Wang<sup>1</sup>; Alexandria L. Sohn<sup>1</sup>; Russell R Kibbe<sup>1</sup>; Daniel C Castro<sup>2</sup>; Jeremy L Norris<sup>2</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>Bruker Daltonics, Billerica, MA
- TP 206 **Comparison of instrumental synchronization modes in mass spectrometric imaging using Orbitrap mass analyzers;** Karl Christian Schäfer<sup>1</sup>; Lars Liebschwager<sup>1</sup>; Kerstin Strupat<sup>2</sup>; Bernhard Spengler<sup>1, 3</sup>; <sup>1</sup>Transmit GmbH, Giessen, Germany; <sup>2</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; <sup>3</sup>Justus Liebig University, Giessen, Germany

### IMAGING MS: INSTRUMENTATION 197-206

- TP 197 **BeamMap: A multi-modal mass spectrometry and electron microscopy imaging instrument on the single-cell scale;** John Sentmanat<sup>1</sup>; Mazdak Taghioskouei<sup>2</sup>; Peter Kottke<sup>1</sup>; Andrei Fedorov<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Trace Matters Scientific, Bethesda, MD

### IMAGING MS: PHARMACEUTICALS, METABOLITES, LIPIDS, AND GLYCANS II 207-229

- TP 207 **Targeted DESI Imaging MS of Drug Distribution and Drug-Induced Liver Injury (DILI) Metabolites from**



## TUESDAY POSTERS

- Methapyrilene in the Male Wistar Rat;** Anthony J Midey<sup>1</sup>; Steven K Lai<sup>1</sup>; Ian D Wilson<sup>2</sup>; Robert S Plumb<sup>1</sup>; Roy Martin<sup>1</sup>; <sup>1</sup>Waters, Milford, MA; <sup>2</sup>Imperial College London, London, United Kingdom
- TP 208 **A lipidomics approach reveals novel lipid changes in skeletal muscles due to muscle hypertrophy and atrophy;** Naoko GOTO-INOUE; Nihon University, Fujisawa, Japan
- TP 209 **Multimodal mass spectrometry imaging reveals biodistributions and biochemical effects of polymeric nanomaterial therapeutic delivery systems;** Jeerapat Dounghawee<sup>1</sup>; Dheeraj K. Agrohia<sup>2</sup>; Teerapong Jantarat<sup>2</sup>; Richard W. Vachet<sup>2</sup>; <sup>1</sup>University of Massachusetts Amherst, Amherst, MA; <sup>2</sup>University of Massachusetts Amherst, Amherst, MA
- TP 210 **Enhancing detection and metabolite annotations in MS imaging using on-tissue chemical derivatization and ion mobility with in-silico prediction of derivatization ;** Dušan Veličković<sup>1</sup>; Kevin Zemaitis<sup>1</sup>; Aiko Barsch<sup>2</sup>; Arne Behrens<sup>2</sup>; Nannan Tao<sup>3</sup>; Nikolas Kessler<sup>2</sup>; Sofie Weinkouff<sup>2</sup>; Christopher Anderton<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>3</sup>Bruker Daltonics, Billerica, MA
- TP 211 **Spatial mapping of N-glycan distributions in a mouse model of primary graft dysfunction post-lung transplantation;** Ariana E Stratton<sup>1</sup>; Hassan H Moussa<sup>2</sup>; Carl Atkinson<sup>2</sup>; Boone M. Prentice<sup>1</sup>; <sup>1</sup>University of Florida Department of Chemistry, Gainesville, FL; <sup>2</sup>University of Florida, Department of Medicine, Gainesville, FL
- TP 212 **Imaging Mass Spectrometry Analysis of Mouse Choroid Plexus;** Michelle Reyzer<sup>1</sup>; Angela Wang<sup>1</sup>; Audra M. Judd<sup>1</sup>; Neil Dani<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- TP 213 **MALDI imaging of glucose in tissue sections by derivatization with betaine aldehyde versus NDEC matrix approach;** Anna Bodzon-Kulakowska<sup>1</sup>; Paulina Kret<sup>1</sup>; Przemysław Mielczarek<sup>1</sup>; Piotr Suder<sup>1</sup>; <sup>1</sup>AGH University of Krakow, Krakow, Poland
- TP 214 **Isomer and Isobar Spatial Traumatic Brain Injury Lipidomics with Desorption Electrospray Ionization Cyclic Ion Mobility Mass Spectrometry Imaging;** Dmitry Leontyev<sup>1</sup>; Hernando Olivos<sup>2</sup>; Bindesh Shrestha<sup>2</sup>; Pooja M Datta Roy<sup>1, 3</sup>; Michelle C. LaPlaca<sup>1, 3</sup>; Facundo M. Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Waters Corporation, Milford, MA; <sup>3</sup>Emory University, Atlanta, GA
- TP 215 **Spatial mapping of plant specialized metabolites using imaging mass spectrometry;** Tetsuya Mori<sup>1</sup>; Noriko Kamiya Takeda<sup>1</sup>; Mai Uzaki<sup>1</sup>; Tomoko Nishizawa<sup>1</sup>; Kiminori Toyooka<sup>1</sup>; Masami Hirai<sup>1</sup>; <sup>1</sup>RIKEN CSRS, Yokohama, Japan
- TP 216 **Unraveling the effects of eribulin pretreatment on docetaxel distribution in tumour xenografts using AP MALDI Mass Spectrometry Imaging;** Alice Passoni<sup>1</sup>; Stefano Mauro Carabellese<sup>1</sup>; Cristina Matteo<sup>1</sup>; Marta Cancelliere<sup>1</sup>; Alessia Lanno<sup>1</sup>; Ugo Cavallaro<sup>2</sup>; Salvatore Lorenzo Renne<sup>3</sup>; Lavinia Morosi<sup>3</sup>; Renzo Bagnati<sup>1</sup>; Massimo Zucchetti<sup>1</sup>; Enrico Davoli<sup>1</sup>; Roberta Frapollini<sup>1</sup>; <sup>1</sup>Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy; <sup>2</sup>European Institute of Oncology IRCCS, Milan, Italy; <sup>3</sup>IRCCS - Humanitas Research Hospital, Rozzano, Italy
- TP 217 **Harnessing the Power of MSI to Improve BASF Formulation and Product Development of Insecticides, Surfactants, and Polymers;** Alanna R Condren<sup>1</sup>; Steven A. DeFiglia<sup>2</sup>; Neven N. Mikawy<sup>2</sup>; James Austin<sup>3</sup>; Kristina Hakansson<sup>2</sup>; Shawn Zhao<sup>1</sup>; <sup>1</sup>BASF Corporation, Wyandotte, MI; <sup>2</sup>University of Michigan Department of Chemistry, Ann Arbor, MI; <sup>3</sup>BASF Corporation, Research Triangle Park, NC
- TP 218 **Spatially Resolved Analysis of Glycosaminoglycans (GAGs) Utilising Trapped Ion Mobility Spectrometry (TIMS);** Anthony J Devlin<sup>1</sup>; C. Logan Mackay<sup>1</sup>; Christopher A Wootton<sup>2</sup>; Felicia Green<sup>1, 3</sup>; Zoltan Takats<sup>1, 4</sup>; <sup>1</sup>Rosalind Franklin Institute, Didcot, United Kingdom; <sup>2</sup>Bruker Daltonics GmbH & Co.KG, Bremen, Germany; <sup>3</sup>University of Oxford, Oxford, United Kingdom; <sup>4</sup>Imperial College London, London, United Kingdom
- TP 219 **Label-Free High-Resolution Molecular Imaging of Sex Steroid Hormones in Zebrafish by Water Cluster Secondary Ion Mass Spectrometry (Cluster SIMS);** Naoko Sano<sup>1</sup>; Elkan Lau<sup>2</sup>; Johanna Von Gerichten<sup>2</sup>; Kate McHardy<sup>3</sup>; Paul Blenkinsopp<sup>3</sup>; Maya Al Sid Cheikh<sup>2</sup>; Melanie Bailey<sup>2</sup>; <sup>1</sup>Ionoptika Ltd, Chandlers Ford, United Kingdom; <sup>2</sup>University of Surrey, School of Chemistry and Chemical Engineering, Guildford, United Kingdom; <sup>3</sup>Ionoptika Ltd, Eastleigh, United Kingdom
- TP 220 **The Effect of Thrombin-Sensitive Platelet-like Particles on the Liver N-Linked Glycome;** Seth M. Eisenberg<sup>1</sup>; Sanika Pandit<sup>2, 3</sup>; Ashley Brown<sup>2, 3</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>FTMS Laboratory for Human Health Research, Raleigh, NC; <sup>2</sup>Joint Department of Biomedical Engineering, North Carolina State University and University of North Carolina-Chapel Hill, Raleigh, NC; <sup>3</sup>Comparative Medicine Institute, Raleigh, NC
- TP 221 **Multimodal Mass Spectrometry Imaging of an Osteosarcoma Multicellular Tumour Spheroid Model to Investigate Drug Induced Response;** Sophie M Pearce<sup>1</sup>; Neil A Cross<sup>1</sup>; David P Smith<sup>1</sup>; Malcolm R Clench<sup>1</sup>; Lucy E Flint<sup>2</sup>; Gregory Hamm<sup>2</sup>; Richard Goodwin<sup>2</sup>; James I. Langridge<sup>3</sup>; Emmanuelle Claude<sup>3</sup>; Laura M Cole<sup>1</sup>; <sup>1</sup>Centre for Mass Spectrometry Imaging, Biomolecular Sciences Research Centre, Sheffield Hallam University, Sheffield, United Kingdom; <sup>2</sup>AstraZeneca, Cambridge, United Kingdom; <sup>3</sup>Waters Corporation, Wilmslow, United Kingdom
- TP 222 **MALDI-MS imaging reveals spatially-localized differences in Ferroptosis-associated lipids in ileum after total body irradiation (TBI);** L.J. Sparvero<sup>1</sup>; Hua Tian<sup>1</sup>; Yulia Tyurina<sup>1</sup>; Michael W Epperly<sup>1</sup>; Joel S. Greenberger<sup>1</sup>; Diane K. Luci<sup>2</sup>; Adam Yasgar<sup>2</sup>; Sandeep Rana<sup>2</sup>; Anton Simeonov<sup>2</sup>; Alexey V. Zakharov<sup>2</sup>; Ganesha Rai<sup>2</sup>; Hülya Bayır<sup>3</sup>; Valerian E. Kagan<sup>1</sup>; <sup>1</sup>University of Pittsburgh, Pittsburgh, PA; <sup>2</sup>National Center for Advancing Translational Sciences (NCATS), Rockville, MD; <sup>3</sup>Columbia University Irving Medical Center, New York, NY
- TP 223 **Evaluating D-Amino Acid Influence on Biofilms in Pseudomonas aeruginosa Lung Infections Under Cystic Fibrosis Conditions through Mass Spectrometry Imaging;** Joenisse M Rosado-Rosa<sup>1</sup>; Dharmeshkumar Parmar<sup>1</sup>; Joshua D ShROUT<sup>2</sup>; Paul W Bohn<sup>2</sup>; Jonathan V Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois Urbana-Champaign, Urbana, IL; <sup>2</sup>University of Notre Dame, Notre Dame, IN
- TP 224 **MALDI IMS of pharmaceutical tablets at 10-µm pixel size without laser oversampling: workflow and surface quality considerations;** Alvaro Santos-Neto<sup>1, 2</sup>; Georgia Charkoftaki<sup>1</sup>; Athina Lisgara<sup>1</sup>; Reza Aalizadeh<sup>1</sup>; Scott Pennino<sup>3</sup>; John Smoliga<sup>3</sup>; Michelle Raikes<sup>3</sup>; Nina Gonnella<sup>3</sup>; Michael Becker<sup>4</sup>; Vladimir V. Papov Jr.<sup>3</sup>; Vasilis Vasiliou<sup>1</sup>; <sup>1</sup>Department of Environmental Health Sciences, Yale School of Public Health, Yale University, New Haven, Connecticut; <sup>2</sup>São Carlos Institute of Chemistry, University of São Paulo, São Carlos 13566-590, SP, Brazil, Brazil; <sup>3</sup>Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, Connecticut; <sup>4</sup>Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach/Riss, Germany
- TP 225 **Mapping nutrient movement, developmental morphogen gradients and electromotive drug delivery with MALDI-TOF Imaging Mass Spectrometry;** Felix Grun<sup>1</sup>; Agatha Kliman<sup>2</sup>; Yi Xi Wu<sup>2</sup>; Matthew Chang<sup>3</sup>; <sup>1</sup>University of California Irvine, Irvine, CA; <sup>2</sup>University of California, Irvine, Irvine, CA; <sup>3</sup>Woodbridge HS, Irvine, California
- TP 226 **Optimization of MALDI-MSI detecting branched-chain amino acids (BCAAs) in Gut-Brain Axis;** Sydni L Chaney<sup>1</sup>; Bandana Bera<sup>2</sup>; Brendan Prideaux<sup>2</sup>; <sup>1</sup>The University of Texas Medical Branch, Galveston, TX; <sup>2</sup>University of Texas Medical Branch at Galveston, Galveston, TX
- TP 227 **Metabolic alterations of Staphylococcus aureus murine bone infection visualized via MALDI Imaging Mass**

## TUESDAY POSTERS

- Spectrometry; Lauren Emmerson<sup>1,2</sup>; Christopher J. Good<sup>1,3</sup>; Madeline E Colley<sup>1,4</sup>; Ali Zahraei<sup>1,5</sup>; Lukasz Migas<sup>1,6</sup>; Raf Van De Plas<sup>1,4,6</sup>; James E. Cassat<sup>7,8,9,10</sup>; Jeffrey M Spraggins<sup>1,2,3,4,5,7,10</sup>; <sup>1</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>2</sup>Chemical and Physical Biology Program, Vanderbilt University, Nashville, Tennessee; <sup>3</sup>Department of Chemistry, Vanderbilt University, Nashville, TN; <sup>4</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>5</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>6</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>7</sup>Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; <sup>8</sup>Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; <sup>9</sup>Department of Biomedical Engineering, Vanderbilt University, Nashville, Tennessee; <sup>10</sup>Vanderbilt Institute for Infection, Immunology and Inflammation, Vanderbilt University School of Medicine, Nashville, Tennessee**
- TP 228 **Analysis and comparison of matched FFPE and fresh frozen tissue by multimodal mass spectrometry imaging; Rory Thomas Steven<sup>1</sup>; Angeliki Christakopoulou<sup>1</sup>; Bin Yan<sup>1</sup>; Ariadna Gonzalez<sup>1</sup>; Josephine Bunch<sup>1,2</sup>; <sup>1</sup>National Physical Laboratory, London, United Kingdom; <sup>2</sup>Imperial College London, London, United Kingdom**
- TP 229 **MALDI Mass Spectrometry Imaging of Aspirin Metabolites and Prostaglandins to Investigate Inflammatory Pathways in Breast Cancer; Taehun Hahn<sup>1,2</sup>; Michael T McMahon<sup>1,3</sup>; Dalton Brown<sup>1,2</sup>; Cole Johnson<sup>1,2</sup>; Caitlin M. Tressler<sup>1,2</sup>; Kristine Glunde<sup>1,2</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore city, MD; <sup>2</sup>Johns Hopkins Applied Imaging Mass Spectrometry (AIMS) Core, Baltimore city, MD; <sup>3</sup>Kennedy Krieger Institute, Baltimore city, MD**
- IMAGING: SPATIALLY-RESOLVED OMICS II**  
230-248
- TP 230 **Applications of all-ion fragmentation for sensitive imaging of esterified fatty acids; Maans Ekeloef<sup>1</sup>; Elena Buglakova<sup>1</sup>; Marteinn Snaebjornsson<sup>2</sup>; Michaela Schwaiger-Haber<sup>3</sup>; Gary J. Patti<sup>3</sup>; Almut Schultze<sup>2</sup>; Theodore Alexandrov<sup>1</sup>; <sup>1</sup>EMBL, Heidelberg, Germany; <sup>2</sup>DKFZ German Cancer Research Center, Heidelberg, Germany; <sup>3</sup>Washington University in Saint Louis, St. Louis, MO**
- TP 231 **Linking MALDI MSI and functional proteomics from heterogeneous tissues: a pixel-by-pixel shotgun spatial proteomic approach; Christopher Kune<sup>1</sup>; Matthieu Hodeige<sup>1</sup>; Maximilien Fleron<sup>2</sup>; Dominique Baiwir<sup>2</sup>; Nor Eddine Sounni<sup>3</sup>; Gauthier Eppe<sup>1</sup>; Gabriel Mazzucchelli<sup>1,2</sup>; <sup>1</sup>Mass Spectrometry Laboratory, MolSys Research Unit, University of Liege, Liege, Belgium; <sup>2</sup>GIGA Proteomics Facility, University of Liège, Liège, Belgium; <sup>3</sup>Laboratory of Tumor and Development Biology, GIGA-Cancer, University of Liege, Liege, Belgium**
- TP 232 **Laser Photobleach Assisted Spatial Proteomics Method for Tissue Sampling in Zebrafish; Julia Ekiert<sup>1</sup>; Beatriz Ibarra<sup>1</sup>; Ankur Saxena<sup>2</sup>; Yu Gao<sup>1</sup>; <sup>1</sup>University of Illinois at Chicago, Chicago, IL; <sup>2</sup>University of Alabama Birmingham, Birmingham, Alabama**
- TP 233 **Open source and scalable spatial reactomics workflow for high resolution mass spectrometry imaging; Miao Yu<sup>1</sup>; Ron Korstanje<sup>2</sup>; Brian Hoffmann<sup>2</sup>; Tim Stodola<sup>2</sup>; Sheng Li<sup>1</sup>; Matt Mahoney<sup>2</sup>; Vivek Philip<sup>2</sup>; Paul Robson<sup>1</sup>; Nadia Rosenthal<sup>2</sup>; <sup>1</sup>The Jackson Laboratory, Farmington, CT; <sup>2</sup>The Jackson Laboratory, Bar Harbor, ME**
- TP 234 **Mass spectrometry imaging of the developing amphibian brain as a tool to discover molecular markers of neurodevelopment; Rikke Poulsen<sup>1,2,3</sup>; Emma M. Field<sup>2</sup>; Haley Kuecks-Winger<sup>2</sup>; Angela M. Jackson<sup>1</sup>; David Goodlett<sup>1,2</sup>; Martin Hansen<sup>3</sup>; Caren C. Helbing<sup>2</sup>; Helena Petrosova<sup>1,2</sup>; <sup>1</sup>University of Victoria Genome BC Proteomics Centre, Victoria, BC; <sup>2</sup>University of Victoria, Department of Biochemistry and Microbiology, Victoria, BC; <sup>3</sup>Aarhus University, Department of Environmental Science, Roskilde, Denmark**
- TP 235 **Untargeted Spatial Metabolomics and Spatial Proteomics on the Same Tissue Section; Gregory W Vandergriff<sup>1</sup>; Marija Veličković<sup>1</sup>; Le Z Day<sup>1</sup>; Sarah M Williams<sup>1</sup>; Bindesh Shrestha<sup>2</sup>; Roy Martin<sup>2</sup>; Christopher R Anderton<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Waters Corporation, Milford, MA**
- TP 236 **Deciphering the Three-Dimensional Biomolecular Distribution in the Alzheimer's Disease Brain: A Multiomic Approach Integrating Immunohistochemistry with MALDI MS Imaging; Kelly H. Lu<sup>1</sup>; Hua Zhang<sup>2</sup>; Gargey B. Yagnik<sup>3</sup>; Mark J. Lim<sup>3</sup>; Kenneth J. Rothschild<sup>3,4</sup>; Andrew J. Schneider<sup>5,6</sup>; Luigi Puglielli<sup>5,6</sup>; Lingjun Li<sup>7,8</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin; <sup>2</sup>University of Wisconsin-Madison School of Pharmacy, Madison, WI; <sup>3</sup>AmberGen Inc., Billerica, MA; <sup>4</sup>Boston University, Department of Physics and Photonics Center, Boston, MA; <sup>5</sup>University of Wisconsin-Madison, Department of Medicine, Madison, WI; <sup>6</sup>University of Wisconsin-Madison, Waisman Center, Madison, WI; <sup>7</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, WI; <sup>8</sup>University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin**
- TP 237 **Decoding Molecular Barcodes of Glomerular Cell Types Through Integrated MALDI IMS and Multiplexed Immunofluorescence Microscopy; Allison B Esselman<sup>1,2</sup>; Léonore Tideman<sup>3</sup>; Felipe A Moser<sup>3</sup>; Lukasz Migas<sup>2,3</sup>; Katerina V Djambazova<sup>2,4</sup>; Madeline E Colley<sup>2,5</sup>; Ellie L Pingry<sup>2,4</sup>; Nathan Heath Patterson<sup>2,5</sup>; Melissa A Farrow<sup>2,5</sup>; Haichun Yang<sup>6,7</sup>; Agnes B Fogo<sup>6,7,8,9</sup>; Mark DeCaestecker<sup>8</sup>; Raf Van De Plas<sup>2,3,5</sup>; Jeffrey M Spraggins<sup>1,2,4,5,6</sup>; <sup>1</sup>Chemistry Department, Vanderbilt University, Nashville, TN; <sup>2</sup>Mass Spectrometry Research Center, Nashville, TN; <sup>3</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>4</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>5</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>6</sup>Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; <sup>7</sup>Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; <sup>8</sup>Division of Nephrology and Hypertension, Vanderbilt University Medical Center, Nashville, TN; <sup>9</sup>Department of Medicine, Vanderbilt University Medical Center, Nashville, TN**
- TP 238 **Coupled MALDI-IMS and Intact Glycoproteomics for Comprehensive Spatial Analysis in Mucinous Tumor Tissues; Sarah C. Lowery<sup>1</sup>; Rachel Stubler<sup>2</sup>; Isabella Tran<sup>1</sup>; Keira E. Mahoney<sup>1</sup>; Georgia Charkoftaki<sup>1</sup>; Vasilis Vasilou<sup>1</sup>; Richard R Drake<sup>2</sup>; Stacy A. Malake<sup>1</sup>; <sup>1</sup>Yale University, New Haven, CT; <sup>2</sup>Medical University of South Carolina, Charleston, SC**
- TP 239 **A preliminary analysis towards the spatial proteomics landscapes of the chemo-refractory related high-grade serous ovarian cancer; Linyuan Fan<sup>1</sup>; Haichao Zhou<sup>1</sup>; Yi Liu<sup>2</sup>; Yang Feng<sup>1</sup>; Guixue Hou<sup>1</sup>; Jianqing Zhu<sup>2</sup>; Siqi Liu<sup>1,3</sup>; <sup>1</sup>University of Chinese Academy of Sciences, Beijing, China; <sup>2</sup>Zhejiang Cancer Hospital, Hangzhou Institute of Medicine (HIM), Chinese Academy of Sciences, Hangzhou, China; <sup>3</sup>BGI-Shenzhen, Shenzhen, China**
- TP 240 **Mapping Molecular Profiles to Cell Types and Neighborhoods through the Integration of MALDI IMS and CODEX Multiplexed IF; Thai H Pham<sup>1,2</sup>; Ellie L Pingry<sup>1,2</sup>; Martin Dufresne<sup>1,3</sup>; Lukasz Migas<sup>1,4</sup>; Felipe A Moser<sup>4</sup>; Madeline E Colley<sup>1,3</sup>; Angela R. S. Kruse<sup>1,2</sup>; Melissa A. Farrow<sup>1,3</sup>; Raf Van De Plas<sup>1,4</sup>; Jeffrey M Spraggins<sup>1,2,3,5,6</sup>; <sup>1</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>2</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, Tennessee; <sup>3</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>4</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>5</sup>Department of**

## TUESDAY POSTERS

- Chemistry, Vanderbilt University, Nashville, TN; <sup>6</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN
- TP 241 **ToF-SIMS-based imaging of unsaturated fatty acyl chain in cell membranes via Pd-catalyzed deuteration;** Yooseong Jeong<sup>1</sup>; Dong-Kyu Lee<sup>1</sup>; <sup>1</sup>College of Pharmacy, Chung-Ang University, Seoul, South Korea
- TP 242 **Mobility-Modulated Sequential Dissociation Analysis Enables Structural Lipidomics in Mass Spectrometry Imaging;** Yao Qian<sup>1</sup>; Zheng Ouyang<sup>1</sup>; Xiaoxiao Ma<sup>2</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>Tsinghua University, Beijing, China
- TP 243 **Exploring the differences in lipid composition of neurons between male and female mice using MALDI-IMS;** Cristina Huergo<sup>1</sup>; Laura De Las Heras-Garcia<sup>2,3,4</sup>; Jone Razquin<sup>3,4,5</sup>; Cristina Miguelez<sup>2,3,4</sup>; Jose A Fernandez<sup>1</sup>; <sup>1</sup>Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Leioa, Spain; <sup>2</sup>Dep of Pharmacology, University of the Basque Country (UPV/EHU), Leioa, Spain; <sup>3</sup>Biocruces Health Research Institute, Neurodegenerative diseases, Barakaldo, Spain; <sup>4</sup>Institut des Maladies Neurodegeneratives IMN, CNRS/University of Bordeaux, Bordeaux, France; <sup>5</sup>Pharmacology, University of the Basque Country (UPV/EHU), Leioa, Spain
- TP 244 **Combining Drug and Targeted Protein Imaging to Uncover Molecular Changes Associated with Cancer Treatment;** Erin H Seeley<sup>1</sup>; Catherine A Kita<sup>2</sup>; Gargey B. Yagnik<sup>2</sup>; Kenneth J. Rothschild<sup>2,3</sup>; Mark J. Lim<sup>2</sup>; Rahul A. Sheth<sup>4</sup>; <sup>1</sup>University of Texas at Austin, Austin, TX; <sup>2</sup>AmberGen Inc., Billerica, MA; <sup>3</sup>Boston University, Department of Physics and Photonics Center, Boston, MA; <sup>4</sup>MD Anderson Cancer Center, Houston, Texas
- TP 245 **Multiplexed targeted imaging of intact proteins in tissue by multi reflecting time of flight (MRT) MALDI-IHC;** Mark Towers<sup>1</sup>; Joel Keelor<sup>2</sup>; Gabriel Stefan Horkovics-Kovats<sup>3</sup>; Steven Pringle<sup>1</sup>; Joanne Ballantyne<sup>1</sup>; Lisa Reid<sup>4</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Waters Corporation, Milford, MA; <sup>3</sup>Hevesy György PhD School, Eötvös Loránd University, Budapest, Hungary; <sup>4</sup>Waters Corporation, Wilmslow, United Kingdom
- TP 246 **MS Imaging for Differential Neuropeptides and Neurotransmitters Colocalization in Cancer borealis Stomogastric Nervous System Resulting from Food Intake;** Wenxin Wu<sup>1</sup>; Penghsuan Huang<sup>1</sup>; Haoran Zhang<sup>1</sup>; Angel E. Ibarra<sup>1</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, WI
- TP 247 **Combined Spatially-Resolved Proteomics and Lipidomics Decipher the Interaction of Collagens and Lipids in Parchment Objects;** Antonia Malissa<sup>1</sup>; Manfred Schreiner<sup>1,2</sup>; Martina Marchetti-Deschmann<sup>1</sup>; <sup>1</sup>TU Wien, Vienna, Austria; <sup>2</sup>Academy of Fine Arts Vienna, Vienna, Austria
- TP 248 **Multimodal Multiplexed Approaches to Assess the Triple-Negative Breast Cancer Microenvironment Linked to Staging and Survival;** Jaclyn B. Dunne<sup>1</sup>; Heather Jensen-Smith<sup>2</sup>; Laura Spruill<sup>1</sup>; Taylor Hulahan<sup>1</sup>; Juliana Gonçalves<sup>3</sup>; Kristina Schwamborn<sup>3</sup>; Mark J. Lim<sup>4</sup>; Gargey B. Yagnik<sup>4</sup>; Kenneth J. Rothschild<sup>4,5</sup>; Anand S. Mehta<sup>1</sup>; Richard R. Drake<sup>1</sup>; Graham Colditz<sup>6</sup>; Marvella E. Ford<sup>1</sup>; Peggi M. Angel<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC; <sup>2</sup>University of Nebraska Medical Center, Omaha, NE; <sup>3</sup>Technical University of Munich (TUM), Munich, Germany; <sup>4</sup>AmberGen Inc, Billerica, MA; <sup>5</sup>Boston University, Department of Physics and Photonics Center, Boston, MA; <sup>6</sup>Washington University in Saint Louis, St. Louis, MO
- TP 250 **Ion Mobility Spectrometry-Mass Spectrometry (IMS-MS) Non-Targeted Analysis Feature Screening: A method for sample classification and feature identification;** Jessie R Chappel<sup>1</sup>; James N. Dodds<sup>2</sup>; Kaylie I Kirkwood-Donelson<sup>3</sup>; Jonathon Fleming<sup>1</sup>; David M Reif<sup>3</sup>; Erin S. Baker<sup>4</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>University of North Carolina - Chapel Hill, Chapel Hill, NC; <sup>3</sup>National Institute of Environmental Health Sciences, Durham, NC; <sup>4</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 251 **Imputation of cancer proteomics data with a deep model that learns jointly from many datasets;** Lincoln J Harris; University of Washington, Seattle, WA
- TP 252 **Bayesian hierarchical linear models for differential protein expression analysis: dealing with data missingness;** Erik T Jansson<sup>1</sup>; Siri Voghera<sup>1</sup>; Måns Magnusson<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden
- TP 253 **Bias in Biomarkers? How to search multiple sample datasets in proteomics database searching software to generate accurate comparisons;** Jessica M Conforti<sup>1</sup>; Constantine C Breus<sup>1</sup>; Charli S Worth<sup>1</sup>; Joseph H Taube<sup>1</sup>; Elyssia S Gallagher<sup>1</sup>; <sup>1</sup>Baylor University, Waco, TX
- TP 254 **Network Analysis as a Supplementary Tool for Exploratory Data Analysis in Modeling Health Outcomes based on Proteomics Data;** Monica Ghaly<sup>1</sup>; Zachary Dwight<sup>1</sup>; Susan Mockus<sup>1</sup>; <sup>1</sup>Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Los Angeles, CA
- TP 255 **A New Approach to Matrix Library Lock Mass Correction (MLLM);** Keith G Richardson<sup>1</sup>; Martin R Green<sup>1</sup>; Christopher J Hughes<sup>1</sup>; Lee A Gethings<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom
- TP 256 **Missingness-informed protein quantification and differential expression analysis;** Mengbo Li; WEHI, Parkville, Australia
- TP 257 **The impact of omics normalization strategies affects grouping and differentiation of biological datasets;** Chi Yen Tseng<sup>1,2</sup>; Erick S. LeBrun<sup>1,2</sup>; Emilio S. Rivera<sup>1,2</sup>; Tara Harvey<sup>1,2</sup>; Joshua D. Breidenbach<sup>1,2</sup>; Brett R. Blackwell<sup>1,2</sup>; Salvador J. Palmisano<sup>1,2</sup>; Grace M. Thornhill<sup>1,2</sup>; Emilia A. Solomon<sup>2</sup>; Claire K. Sanders<sup>3</sup>; Marc Alvarez<sup>2</sup>; Kes A. Luchini<sup>1,2</sup>; Abigale S Mikolitis<sup>1,2</sup>; Zachary J. Sasiene<sup>1,2</sup>; Ethan M. McBride<sup>1,2</sup>; Austin R. Anderson<sup>1,2</sup>; Lauren K. Heine<sup>1,2</sup>; Jessica A. Salguero<sup>1,2</sup>; Francisca E. Rodriguez<sup>1,2</sup>; Phillip M. Mach<sup>1,2</sup>; Trevor G. Glaros<sup>1,2</sup>; <sup>1</sup>Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>3</sup>Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM
- TP 258 **JUMPsem: Enzyme Activity Inference with Structural Equation Modeling;** Dehui Kong<sup>1</sup>; Aijun Zhang<sup>1</sup>; Ling Li<sup>1</sup>; Zuofei Yuan<sup>2</sup>; Yingxue Fu<sup>3</sup>; Long Wu<sup>2</sup>; Ashutosh Mishra<sup>2</sup>; Anthony High<sup>2</sup>; Junmin Peng<sup>2</sup>; Xusheng Wang<sup>1,2</sup>; <sup>1</sup>University of Tennessee Health Science Center, Memphis, TN; <sup>2</sup>St. Jude Children's Research Hospital, Memphis, TN; <sup>3</sup>St. Jude Children's Research Hospital, Memphis, TN
- TP 259 **A novel statistical similarity score using replicate electron-ionization mass spectra;** Amudhan Krishnaswamy-Usha<sup>1</sup>; Briana A. Capistran<sup>1</sup>; Edward Sisco<sup>1</sup>; Anthony J. Kearsley<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, Gaithersburg, MD
- TP 260 **CPred: Charge State Prediction for Modified and Unmodified Peptides in Electrospray Ionization;** Frédérique Vilenne<sup>1</sup>; Annelies Agten<sup>1</sup>; Simon Appeltans<sup>1</sup>; Dirk Valkenborg<sup>1</sup>; <sup>1</sup>Hasselt University, Diepenbeek, Belgium
- TP 261 **Characterization of Peptide Ancestry Informative Markers in Lung Adenocarcinomas from Individuals of European and East Asian Ancestry;** Tamara Abulez<sup>1</sup>; Jeremy L Loffredo<sup>1</sup>; Christopher M Tarney<sup>1</sup>; Timothy D O'Connor<sup>2</sup>; Brian L Hood<sup>1</sup>; Glendon J Parker<sup>3</sup>; Kathleen M

### INFORMATICS: ALGORITHMS AND STATISTICAL ADVANCES 249-283

- TP 249 **PyViscount: Flexible Validation of FDR Estimation Methods by Search Space Partition Into Countable Sets;**

## TUESDAY POSTERS

- Darcy<sup>1</sup>; Neil T Phippen<sup>1</sup>; George L Maxwell<sup>1</sup>; Thomas P Conrads<sup>1</sup>; Nicholas W. Bateman<sup>1</sup>; <sup>1</sup>Women's Health Integrated Research Center, Annandale, VA; <sup>2</sup>Program in Personalized and Genomic Medicine, University of Maryland School of Medicine, Baltimore, MD; <sup>3</sup>University of California, Davis, Davis, CA
- TP 262 **JUMP-BREAD: A User-Friendly R Shiny Tool for Streamlining Block Randomization in the Experimental Analysis and Design of Proteomics Studies;** Yingxue Fu<sup>1</sup>; Zuofei Yuan<sup>2</sup>; Long Wu<sup>2</sup>; Xusheng Wang<sup>2</sup>; Junmin Peng<sup>2</sup>; Anthony High<sup>2</sup>; <sup>1</sup>St Jude Children's Research Hospital, Memphis, TN; <sup>2</sup>St. Jude Children's Research Hospital, Memphis, TN
- TP 263 **Assessment of false discovery rate control in tandem mass spectrometry analysis using entrapment;** Bo Wen<sup>1</sup>; Jack Freestone<sup>2</sup>; Michael J. MacCoss<sup>1</sup>; William S Noble<sup>1,3</sup>; Uri Keich<sup>2</sup>; <sup>1</sup>Department of Genome Sciences, University of Washington, Seattle, Washington; <sup>2</sup>Department of Statistics, University of Sydney, Sydney, Australia; <sup>3</sup>Paul G. Allen School of Computer Science and Engineering, University of Washington, Seattle, WA
- TP 264 **A new statistical model for open search localization;** Daniel J Geiszler<sup>1</sup>; Nurhan Ozlu<sup>1,2</sup>; <sup>1</sup>Department of Molecular Biology and Genetics, Koç University, Istanbul, Turkey; <sup>2</sup>Koç University Research Center for Translational Medicine (KUTTAM), Koç University, Istanbul, Turkey
- TP 265 **NovoCert: Statistical validation of de novo peptide sequencing;** Shanji Zhang<sup>1</sup>; Seunghyuk Choi<sup>2</sup>; Seungjin Na<sup>3</sup>; Eunok Paek<sup>1,4</sup>; <sup>1</sup>Department of Computer Science, Hanyang University, Seoul, South Korea; <sup>2</sup>Baylor College of Medicine, Houston, TX; <sup>3</sup>Korea Basic Science Institute, Cheongju, South Korea; <sup>4</sup>Institute for Artificial Intelligence Research, Hanyang University, Seoul, South Korea
- TP 266 **ProtPipe2.0: A Multifunctional Data Analysis Pipeline for Proteomics, pSILAC and Peptidomics;** Ziyi Li; NIH, Bethesda, MD
- TP 267 **Considerations Before Log-Transforming LC-MS Omics Data;** Matthew J Keller<sup>1,2</sup>; Steven Tavis<sup>1,2</sup>; Robert L Hettich<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of Tennessee Knoxville, Knoxville, TN
- TP 268 **Assessing the Effects of Retention-Time Alignment on Protein Abundance in Proteomics Database Searching;** Constantine C Breus<sup>1</sup>; Jessica M Conforti<sup>1</sup>; Elyssia S Gallagher<sup>1</sup>; <sup>1</sup>Baylor University, Waco, TX
- TP 269 **Beyond ion-intensity prediction: an end-to-end model for Peptide-Spectrum matching;** Maximilien Burg<sup>1</sup>; Jure Zbontar<sup>1</sup>; Juan L. Restrepo<sup>2</sup>; Shamil Urzabakhtin<sup>3</sup>; Jurgen Cox<sup>2</sup>; Peter Cimermancic<sup>1</sup>; <sup>1</sup>Tesorai, San Diego, CA; <sup>2</sup>Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Munich, Germany; <sup>3</sup>Computational Systems Biochemistry Research Group, Max Planck Institute of Biochemistry, Munich, Germany
- TP 270 **Evaluating the Performance of ProteoMixture, a Proteomics-Based Cell Deconvolution Tool in Pan-Cancer Data for > 1000 Patient Tumors;** Joshua P Schaaaf<sup>1</sup>; Tamara Abulez<sup>1</sup>; Pang-ning Teng<sup>1</sup>; Brian L Hood<sup>1</sup>; Kelly A Conrads<sup>1</sup>; Tracy J Litzl<sup>1</sup>; Allison L Hunt<sup>1</sup>; Kathleen M Darcy<sup>1</sup>; Neil T Phippen<sup>1</sup>; Thomas P Conrads<sup>1</sup>; Nicholas W Bateman<sup>1</sup>; <sup>1</sup>Women's Health Integrated Research Center, Annandale, VA
- TP 271 **MultiplexMixer: An Enabling Utility for Rational Sample Randomization for Multiplexed, Quantitative Proteomic Workflows;** Jordan A Driscoll<sup>1</sup>; Tamara Abulez<sup>1</sup>; Kelly A Conrads<sup>1</sup>; Brian L Hood<sup>1</sup>; Kathleen M Darcy<sup>1</sup>; Christopher M Tarney<sup>1</sup>; Neil T Phippen<sup>1</sup>; George L Maxwell<sup>1</sup>; Nicholas W. Bateman<sup>1</sup>; Thomas P Conrads<sup>1</sup>; <sup>1</sup>Women's Health Integrated Research Center, Annandale, VA
- TP 272 **Sin.R: A SAINT-like AP-MS protein-interaction score implemented in R;** Manor Askenazi<sup>1</sup>; Jackeline Ponce<sup>2</sup>; Beatrix Ueberheide<sup>2</sup>; <sup>1</sup>Biomedical Hosting LLC, Arlington, MA; <sup>2</sup>NYU Grossman School of Medicine, New York, NY
- TP 273 **Preserving Full-Profile Information in Analysis and Compression of Imaging Mass Spectrometry Data by Sparsity-Aware Low-Rank Matrix Factorization;** Roger A.R. Moens<sup>1</sup>; Lukasz Migas<sup>1</sup>; Jacqueline Van Ardenne<sup>2,3</sup>; Cody Marshall<sup>2,4</sup>; David Reeves<sup>2,5</sup>; Ölöf Isberg<sup>2,5</sup>; Martin Dufresne<sup>2,6</sup>; Jeffrey M. Spraggins<sup>2,3,4,5,6</sup>; Raf Van De Plas<sup>1,2,6</sup>; <sup>1</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>2</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>3</sup>Department of Chemistry, Vanderbilt University, Nashville, TN; <sup>4</sup>Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN; <sup>5</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>6</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN
- TP 274 **High Dimensional Consensus spectra for Single-Compound Forensic Drug Discrimination;** Wencheng Zhong<sup>1</sup>; Briana A. Capistran<sup>2</sup>; Amudhan Krishnaswamy Usha<sup>2</sup>; Edward Sisco<sup>2</sup>; Anthony J. Kearsley<sup>2</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>National Institute of Standards and Technology, Gaithersburg, MD
- TP 275 **Evaluating statistical methods and experimental designs for chemoproteomics experiments;** Sarah Szvetcz<sup>1</sup>; Pierre Jean Beltran<sup>2</sup>; Joel Federspiel<sup>3</sup>; Denise Field<sup>2</sup>; Robert J Seward<sup>3</sup>; Hyunsuk Suh<sup>3</sup>; Devon Kohler<sup>1</sup>; Liang Xue<sup>2</sup>; Olga Vitek<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Pfizer, Inc, Cambridge, MA; <sup>3</sup>Pfizer Inc., Andover, MA
- TP 276 **MAPLE: A Pipeline for Mapping Ancestry-linked Protein Quantitative Trait Loci in Proteogenomic Data;** Satishkumar Ranganathan Ganakammal<sup>1</sup>; Jordan A Driscoll<sup>1</sup>; Tamara Abulez<sup>1</sup>; Christopher M Tarney<sup>1</sup>; Brian L Hood<sup>1</sup>; Kathleen M Darcy<sup>1</sup>; Neil T Phippen<sup>1</sup>; Ayman Al-Hendy<sup>2</sup>; George L Maxwell<sup>1</sup>; Thomas P Conrads<sup>1</sup>; Nicholas W. Bateman<sup>1</sup>; <sup>1</sup>Women's Health Integrated Research Center, Annandale, VA; <sup>2</sup>University of Chicago, Chicago, IL
- TP 277 **Spectral similarity based on Siamese network model embeddings broadly outperforms standard cosine similarities on molecular networking tasks;** Gennady Voronov<sup>1</sup>; Daniel Ence<sup>1</sup>; Joe Rokicki<sup>1</sup>; <sup>1</sup>Enveda Biosciences, Boulder, CO
- TP 278 **Run-to-run retention time alignment improves peak picking in Skyline;** Nicholas Shulman<sup>1</sup>; Deanna L. Plubell<sup>1</sup>; Brendan MacLean<sup>1</sup>; Michael J. MacCoss<sup>1</sup>; <sup>1</sup>University of Washington - Genome Sciences, Seattle, WA
- TP 279 **Methods for Automated Calibration and Elemental Composition Assignment of Complex Mixtures: PyC2MC Updates;** Ryan P Rodgers<sup>1</sup>; Christopher L Hendrickson<sup>2,3</sup>; Christopher Holder Montenegro<sup>2,4</sup>; Martha L Chacon-Patino<sup>2,3</sup>; Alvaro J Tello Rodriguez<sup>2,4</sup>; Christopher Rüger<sup>5</sup>; Germain Salvato Vallverdu<sup>3,6</sup>; <sup>1</sup>Nat'l High Magnetic Field Lab, Tallahassee, FL; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, Florida; <sup>3</sup>International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France; <sup>4</sup>Florida State University, Tallahassee, FL; <sup>5</sup>University of Rostock, Rostock, Germany; <sup>6</sup>Université de Pau et des Pays de l'Adour, Pau, France
- TP 280 **Construction of large collections of reference precursor retention times and modes across multiple tissue types;** Duong Nguyen<sup>1,2,3</sup>; Nuno Bandeira<sup>1,2,3,4</sup>; <sup>1</sup>University of California San Diego, La Jolla, CA; <sup>2</sup>Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; <sup>3</sup>Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; <sup>4</sup>Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA
- TP 281 **Using First Principles to Develop Population Scale Peak Picking Software for the Genome Era: The I.A.A Suite;** Allen Hubbard<sup>1</sup>; Louis Connelly<sup>1</sup>; Rijan Dhakal<sup>1</sup>; Shrikaar Kambhampati<sup>1</sup>; Ivan Baxter<sup>1</sup>; <sup>1</sup>Donald Danforth Plant Science Center, Saint Louis, MO

## TUESDAY POSTERS

- TP 282 **Implementation of De Novo Sequencing Methods Based on a Visual Acuity Ion Classifier for Top-down, Middle-down, and Bottom-up Fragmentation Spectra;** Blake Hakilla<sup>1</sup>; Stephanie Sturgeon<sup>1</sup>; Timothy Djang<sup>2</sup>; Alex Gavrilenko<sup>2</sup>; Jhenya Gavrilenko<sup>2</sup>; Stelios Gkegkas<sup>2</sup>; Panos Iatrou<sup>2</sup>; Rachel Franklin<sup>1</sup>; Yury V. Vasilev<sup>3</sup>; Diana Oppenheimer<sup>1</sup>; Joseph Meeuswen<sup>1</sup>; Adrian L Guthals<sup>1</sup>; <sup>1</sup>Agilent Technologies, Corvallis, Oregon; <sup>2</sup>Devicepros, Boston, USA, MA; <sup>3</sup>Agilent Technologies, Santa Clara, CA
- TP 283 **Accelerated Analysis of Structurally Related Components in Complex Samples;** Anne Marie Smith<sup>1</sup>; Alexander Lishchuk<sup>1</sup>; Alexander Sakharov<sup>1</sup>; <sup>1</sup>ACD/Labs, Toronto, ON
- INSTRUMENTATION: GENERAL**  
**284-299**
- TP 284 **Time-resolved characterization and analysis of pulsed ion sources by synchronized oaTOF-MS;** Franziska Schuler<sup>1</sup>; Joshua Rieger<sup>1</sup>; Maja Hammelrath<sup>1</sup>; Sanna Benter<sup>1</sup>; Hendrik Kersten<sup>1</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany
- TP 285 **Interfacing a Compact Capillary Liquid Chromatograph to a Small Footprint Triple Quadrupole Mass Spectrometer;** Serguei V. Calugaru<sup>1</sup>; Elisabeth P. Gates<sup>1</sup>; W. Raymond West<sup>1</sup>; Milton L. Lee<sup>1</sup>; Charmion I. E. Cruickshank-Quinn<sup>2</sup>; Wendi A. Hale<sup>2</sup>; David A. Jarvis<sup>2</sup>; <sup>1</sup>Axend, Provo, UT; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- TP 286 **Orbitrap-based Charge Detection Mass Spectrometry using an External Data Acquisition and Processing System;** Yury Tsybin<sup>1</sup>; Konstantin O. Nagornov<sup>1</sup>; Natalia Gasilova<sup>2</sup>; Laure Menin<sup>2</sup>; Anton N. Kozhinov<sup>1</sup>; <sup>1</sup>Spectroswiss, Lausanne, Switzerland; <sup>2</sup>Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
- TP 287 **Operating electrodynamic ion funnels in wide m/z transmission mode for simultaneous analysis of labile and non-labile analytes;** Peter Weidner<sup>1</sup>; Behrooz Zekavat<sup>1</sup>; Anabel Fandino<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- TP 288 **Gated trapped ion mobility spectrometry coupled to Fourier transform ion cyclotron resonance mass spectrometer to characterize future green fuels;** Julien Maillard<sup>1,2</sup>; Gregory Brabeck<sup>3</sup>; Alina Theisen<sup>3</sup>; Christopher Ruger<sup>2</sup>; Pierre Giusti<sup>1,2,4</sup>; Carlos AFONSO<sup>2,4</sup>; Christopher A Wootton<sup>3</sup>; <sup>1</sup>TotalEnergies, Harfleur, France; <sup>2</sup>International Joint Laboratory—iC2MC: Complex Matrices Molecular Characterization, TRTG, BP 27, 76700 Harfleur, France, Harfleur, France; <sup>3</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; <sup>4</sup>University of Rouen-Normandy, Mont-Saint-Aignan, France
- TP 289 **The benefit of high power and pressure in ultra-violet photodissociation (UVPD);** Mircea Guna<sup>1</sup>; Pavel Ryumin<sup>1</sup>; Anjali Chelur<sup>1</sup>; Nick Albeau<sup>1</sup>; Yves Le Blanc<sup>2</sup>; <sup>1</sup>SCIEX, Concord, ON; <sup>2</sup>SCIEX, Concord, On, ON
- TP 290 **Practical Quadrupole Theory: Characterization of Quadrupole Performance for Various Rod Lengths, with and without Pre-Filters;** Luke Metzler<sup>1</sup>; Randall E Pedder<sup>1</sup>; Jacob Pasko<sup>1</sup>; Alex Miscovich<sup>1</sup>; <sup>1</sup>Ardara Technologies, Ardara, PA
- TP 291 **Management of a Centralized Gas Generation System in a Clinical LC-MS/MS Lab over an 11-Year Growth Period;** Brett Holmquist; <sup>1</sup>Labcorp, Calabasas Hills, CA
- TP 292 **Multivendor and Multiplatform Comparison of Linearity and Sensitivity in Mass Spectrometry Imaging;** Andrew Bowman<sup>1</sup>; Nari Talaty<sup>1</sup>; David Wagner<sup>1</sup>; Junhai Yang<sup>1</sup>; <sup>1</sup>AbbVie, Inc., North Chicago, IL
- TP 293 **Different extraction mechanisms of the mass-selective axial ejection from linear quadrupole ion trap;** Fulong Deng; <sup>1</sup>Sichuan University, Chengdu, China
- TP 294 **Ion transmission characterization through a dual-field converging multipole ion guide;** Haopeng Wang<sup>1</sup>; Laura L Pollum<sup>1</sup>; Patrick M Batoon<sup>1</sup>; <sup>1</sup>Agilent Technologies Inc., Santa Clara, CA
- TP 295 **Triple Quadrupole Mass Spectrometer Performance: Evaluation and Mitigation of Charging;** Jason D. White<sup>1</sup>; Michael V. Ugarov<sup>1</sup>; Hans Schweingruber<sup>1</sup>; Charles E. Maxey<sup>1</sup>; Neloni R. Wijeratne<sup>1</sup>; Claudia P.B. Martins<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA
- TP 296 **Mass resolved “line-writing” and targeted area coverage for ion soft-landing;** Michael Espenship<sup>1</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- TP 297 **Development of oxygen attachment dissociation (OAD)-TOF system incorporating a modified collision cell;** Yuta Miyazaki<sup>1</sup>; Tomoya Kudo<sup>1</sup>; Ryosuke Nara<sup>1</sup>; Hidenori Takahashi<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan
- TP 298 **Toward the Quantification of Ion Losses in Non-Linear Quadrupole Ion Guides in a Folded-Layout Triple Quadrupole Mass Spectrometer;** Matthias Lorenz<sup>1</sup>; Anna Kornilova<sup>1</sup>; Adrian Maclean<sup>1</sup>; Tak Shun Cheung<sup>1</sup>; Hamid Badiei<sup>1</sup>; <sup>1</sup>PerkinElmer, Woodbridge, ON
- TP 299 **Addressing sustainability in the laboratory through the evaluation of energy consumption of a prototype benchtop LC-MS platform;** Rachel J Sanig<sup>1</sup>; Andrew Whately<sup>1</sup>; Matthew Gibbs<sup>1</sup>; Lee A Gethings<sup>1</sup>; Gunnar Weibchen<sup>2</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Waters Corporation, Eschborn, Germany
- ION MOBILITY: APPLICATIONS II**  
**300-319**
- TP 300 **Development of a Cyclic Ion Mobility Spectrometry-Mass Spectrometry (cIMS-MS)-Based Collision Cross Section Database of Permethylated Human Milk Oligosaccharides;** Sanaz C Habibi<sup>1</sup>; Gabe Nagy<sup>1</sup>; <sup>1</sup>University of Utah, Salt Lake City, UT
- TP 301 **Separation of New Psychoactive Substances and Xylazine Metabolite Isomers using SLIM High-Resolution Ion Mobility-Mass Spectrometry (HRIM-MS);** Ralph Aderorho<sup>1</sup>; Christopher Donald Chouinard<sup>1</sup>; <sup>1</sup>Clemson University, Clemson, SC
- TP 302 **Trapped ion mobility spectrometry for high-throughput directed evolution screening of  $\alpha$ -ketoglutarate dependent dioxygenases;** Robert A. Shepherd<sup>1</sup>; Austin R. Hopiavuori<sup>1</sup>; Melanie C. Jones<sup>1</sup>; Alex J. Tabag<sup>1</sup>; Conrad A. Fihn<sup>1</sup>; Shaun M. McKinnie<sup>1</sup>; Laura M Sanchez<sup>1</sup>; <sup>1</sup>UC Santa Cruz, Santa Cruz, CA
- TP 303 **Structural Characterization of Isomeric Reaction Products using High-Resolution SLIM Ion Mobility and Computational Approaches;** Walker N Hodges<sup>1</sup>; Shadrack W. Lucas<sup>1</sup>; Ralph Aderorho<sup>1</sup>; Christopher Donald Chouinard<sup>1</sup>; <sup>1</sup>Clemson University, Clemson, SC
- TP 304 **Optimization of Liquid Chromatography Trapped Ion Mobility Tandem Mass Spectrometry for Collagenase Proteomics;** Jade K. Macdonald<sup>1</sup>; Stephen C. Zambrycki<sup>1</sup>; Richard R Drake<sup>1</sup>; Peggi M Angel<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC
- TP 305 **Compilation of a Polysorbate CCS Database from Drift Tube and Traveling Wave Structures for Lossless Ion Manipulations Ion Mobility Measurements;** Kyle E Lira<sup>1</sup>; Jody C May<sup>1</sup>; John A McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- TP 306 **Ion mobility-based approaches for the separation and identification of chiral active pharmaceutical ingredients;** Valeria Guidolin<sup>1</sup>; Jody C. May<sup>2</sup>; Almary Chacon<sup>1</sup>; Benjamin K. Blakley<sup>2</sup>; Eric Dybeck<sup>1</sup>; John A. McLean<sup>2</sup>; <sup>1</sup>Pfizer, Groton; <sup>2</sup>Vanderbilt University, Nashville, TN
- TP 307 **Evaluation of Chiral Selection Strategies with Ion Mobility-Mass Spectrometry for Differentiating Enantiomers of Drug and Drug-Like Compounds;** Benjamin K Blakley<sup>1</sup>; Jody C May<sup>1</sup>; Valeria Guidolin<sup>2</sup>; John A McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Pfizer, Groton
- TP 308 **Assessing the Additivity of Mass-Distribution Based Shifts in High-Resolution Cyclic Ion Mobility Separations;** Noah D Roberts<sup>1</sup>; David L Williamson<sup>1</sup>; Gabe Nagy<sup>1</sup>; <sup>1</sup>University of Utah, Salt Lake City, UT

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- TP 309 **Ion Mobility and Collision Induced Unfolding Characterize Metal-Dependent Nucleic Acid-Protein Interactions;** Caela P Fedraw<sup>1,2</sup>; Anna G Anders<sup>1</sup>; Nicholas J Rossiter<sup>3</sup>; Stephen A DeAngelo<sup>4</sup>; Markos Koutmos<sup>1, 5, 6</sup>; Costas A Lyssiotis<sup>7, 8</sup>; Yatrik M Shah<sup>8, 9</sup>; Brandon T. Ruotolo<sup>10</sup>; <sup>1</sup>Department of Chemistry, University of Michigan, Ann Arbor, MI; <sup>2</sup>Michigan Medicine Post-baccalaureate Research Education Program, University of Michigan, Ann Arbor, MI; <sup>3</sup>Cellular and Molecular Biology Program, University of Michigan Medical School, Ann Arbor, MI; <sup>4</sup>Doctoral Program in Cancer Biology, University of Michigan, Ann Arbor, MI; <sup>5</sup>Program in Biophysics, University of Michigan, Ann Arbor, MI; <sup>6</sup>Program in Chemical Biology, University of Michigan, Ann Arbor, MI; <sup>7</sup>Department of Molecular and Integrative Physiology, University of Michigan Medical School, Ann Arbor, MI; <sup>8</sup>Department of Internal Medicine, University of Michigan, Ann Arbor, MI; <sup>9</sup>University of Michigan Rogel Cancer Center, University of Michigan, Ann Arbor, MI; <sup>10</sup>Department of Chemistry, University of Michigan, Ann Arbor, Michigan
- TP 310 **Rapid identification and quantification of dihydroxyacetophenone positional isomers by ion mobility spectrometry time-of-flight mass spectrometry and theoretical calculations;** Chuan-Fan Ding<sup>1</sup>; Yinghua Yan<sup>1</sup>; Baichun Wang<sup>1</sup>; Xiaohui Huang<sup>1</sup>; <sup>1</sup>Ningbo University, Ningbo, China
- TP 311 **High-Resolution Ion Mobility Analysis of Isomeric Bile Acids Using Structures for Lossless Ion Manipulations (SLIM) IM-MS;** Emmaleigh D Efrid<sup>1</sup>; Makenna Hoover<sup>1</sup>; Terra Pettit-Bacovin<sup>1</sup>; Ashlee Wedge<sup>1</sup>; Christopher D. Chouinard<sup>1</sup>; <sup>1</sup>Clemson University, Clemson, SC
- TP 312 **Targeted Head Group Identification for Characterizing Glycolipid Isomers Using Cyclic Ion Mobility Separations;** Cameron N Naylor<sup>1</sup>; Gabe Nagy<sup>1</sup>; <sup>1</sup>University of Utah, Department of Chemistry, Salt Lake City, UT
- TP 313 **Ion mobility separation of marine natural products: Characellides from the deep sea sponge Characella pachastrelloides;** Sarah Dowd<sup>1</sup>; Sam Afoullouss<sup>2</sup>; Jennifer Netjes<sup>2</sup>; Bill J Baker<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>University of South Florida, Tampa, FL
- TP 314 **Isolating the Effect of Moments of Inertia in High-Resolution Ion Mobility Spectrometry-Mass Spectrometry;** David L. Williamson<sup>1</sup>; Noah D Roberts<sup>1</sup>; Haisley Windsor<sup>1</sup>; Gabe Nagy<sup>1</sup>; <sup>1</sup>University of Utah, Department of Chemistry, Salt Lake City, UT
- TP 315 **Method Development and Characterization of PFAS Compounds Using Structures for Lossless Ion Manipulations (SLIM) IM-MS;** Heidi Sabatini<sup>1</sup>; Terra Pettit-Bacovin<sup>1</sup>; Ralph Aderorho<sup>1</sup>; Christopher D. Chouinard<sup>1</sup>; <sup>1</sup>Clemson University, Clemson, SC
- TP 316 **Structure elucidation of divarasib is mediated by alternative activation and separation strategies;** Chris M Crittenden<sup>1</sup>; Marcelino Varona<sup>1</sup>; Daniel P. Dobson<sup>1</sup>; José G. Napolitano<sup>1</sup>; <sup>1</sup>Genentech Inc., South San Francisco, CA
- TP 317 **Cyclic Peptide Soft Spot Identification (SSID) by High-resolution Ion Mobility Mass Spectrometry (HRIM-MS) using label-free and isotope-labeled dimethylation strategies;** Komal Kedia<sup>1</sup>; Maria Fawaz<sup>1</sup>; Congliang Sun<sup>1</sup>; Yu Feng<sup>1</sup>; Athanasia Qirjollari<sup>1</sup>; Hubert Josien<sup>1</sup>; Kara M Pearson<sup>1</sup>; Raymond J. Gonzalez<sup>1</sup>; Lisa O'Callaghan<sup>1</sup>; Mark T. Cancilla<sup>1</sup>; Weixun Wang<sup>1</sup>; Daniel S. Spellman<sup>1</sup>; <sup>1</sup>Merck Sharp & Dohme LLC, West Point, PA
- TP 318 **Enhanced detection and quantitation of targeted metabolites through native ion mobility-mass spectrometry and collisional ligand ejection;** Michael R Armbruster<sup>1</sup>; Brandon T Ruotolo<sup>1</sup>; <sup>1</sup>University of Michigan Department of Chemistry, Ann Arbor, MI
- TP 319 **Study on the aggregation of alpha-synuclein peptides and stable oligomeric conformations using IM-MS and MD simulations;** Zhiyuan Zhu<sup>1</sup>; Yilei Li<sup>1</sup>; Michael T. Bowers<sup>1</sup>; <sup>1</sup>UCSB, Santa Barbara, CA

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- TP 320 **Prediction of isotopologue concentration from an AI model for unlabelled analytes: The foundation for absolute quantitation in metabolomic flux analyses;** Joshua Lauterbach<sup>1</sup>; Ana S.H. Costa<sup>1</sup>; Devesh Shah<sup>1</sup>; Luke S. Ferro<sup>1</sup>; Steven B. Hooper<sup>1</sup>; Jack Howland<sup>1</sup>; Jefferson G. Pruyne<sup>1</sup>; Timothy Kassis<sup>1</sup>; Jennifer M. Campbell<sup>1</sup>; <sup>1</sup>Matterworks, Inc., Somerville, MA
- TP 321 **13C-metabolic flux analysis using GC-MS reveals metabolic rewiring in HL-60 neutrophil-like cells through differentiation and immune stimulation;** Takeo Taniguchi<sup>1</sup>; Nobuyuki Okahashi<sup>1</sup>; Fumio Matsuda<sup>1</sup>; <sup>1</sup>Osaka university, Osaka, Japan
- TP 322 **An Ultra-High Throughput Cell-Based Mass Spectrometry Flux Assay as an in-situ Screening Strategy.;** Daniel P Downes<sup>1</sup>; Christopher M Barbieri<sup>1</sup>; Lisa M. Kopcho<sup>1</sup>; David Connors<sup>1</sup>; Madhu Sudhan Ravindran<sup>2</sup>; Wilson Z. Shou<sup>1</sup>; Andrew D. Wagner<sup>1</sup>; Brian J. Arey<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb, Princeton, NJ; <sup>2</sup>Syngene, Bangalore, India
- TP 323 **Application of multiple isotope pattern searches for in-depth plant metabolism determination;** Chris Brown<sup>1</sup>; Jeffrey R Gilbert<sup>1</sup>; Yelena Adelfinskaya<sup>1</sup>; Eva Duchoslav<sup>2</sup>; Yves LeBlanc<sup>2</sup>; <sup>1</sup>Corteva Agriscience, Indianapolis, IN; <sup>2</sup>SCIEX, Concord, ON
- TP 324 **3D-printed stackable air-liquid interface platform with paper-based cell culture enables isotopic flux analysis of cancer volatiles via HS-SPME/GC-MS;** Hyoieong Lee<sup>1</sup>; Dong-kyu Lee<sup>1</sup>; <sup>1</sup>College of Pharmacy, Chung-Ang University, Seoul, South Korea
- TP 325 **Top-Simple Light Isotope Metabolic (SLIM)-Labeling, a unique method for LC-MS-based quantification of intact proteins in complex samples.;** Jean-Michel CAMADRO<sup>1</sup>; Denis MESTIVIER<sup>2</sup>; Nicolas SENECAUT<sup>3</sup>; Alexia LOURENCO<sup>4</sup>; Victor COCHARD<sup>1</sup>; Marie LEY<sup>1</sup>; Véronique LEGROS<sup>1</sup>; Guillaume CHEVREUX<sup>1</sup>; <sup>1</sup>Institut Jacques Monod CNRS, Paris, France; <sup>2</sup>Université Paris-Est Créteil, Créteil, France; <sup>3</sup>Rijksuniversiteit Groningen, Groningen, Netherlands; <sup>4</sup>Inovaron, Paris, France

LC/MS: SAMPLE PREPARATION I  
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- TP 326 **Facilitating large-scale proteomics by combining automated sample preparation with short gradient LC-MS acquisitions;** Luca Sandro Räss<sup>1</sup>; Sandra Schär<sup>1</sup>; Roland Bruderer<sup>1</sup>; Christopher Below<sup>1</sup>; Ino Karemaker<sup>1</sup>; Lukas Reiter<sup>1</sup>; <sup>1</sup>BiognoSYS, Schlieren, Switzerland
- TP 327 **Simplified Detergent Facilitated End-to-End Automation of LC-MS Biopharmaceutical Peptide Mapping;** Jason L. Richardson<sup>1</sup>; Zhongqi Zhang<sup>1</sup>; <sup>1</sup>Amgen, Thousand Oaks, CA
- TP 328 **Broad chemical space sample preparation and sensitive LC-MS/MS for high-throughput exposomics;** Yunyun GU<sup>1</sup>; Maren Kirchner<sup>1</sup>; Caroline Helen Johnson<sup>2</sup>; Benedikt Warth<sup>1</sup>; <sup>1</sup>University of Vienna, Vienna, Austria; <sup>2</sup>Yale University, New Haven, CT
- TP 329 **Bringing Simplicity into Plasma Proteomics by Applying a Fast, High-Throughput and Standardized Automation Platform;** Fabian Wendt<sup>1</sup>; Claudia Martelli<sup>2</sup>; Zehan Hu<sup>3</sup>; Andreas Schmidt<sup>4</sup>; Christopher Below<sup>5</sup>; Roland Bruderer<sup>6</sup>; Katrin Hartinger<sup>3</sup>; Gary Kruppa<sup>8</sup>; Nils A. Kulak<sup>3</sup>; Manuel Bauer<sup>1</sup>; <sup>1</sup>Tecan, Männedorf, Switzerland; <sup>2</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>3</sup>PreOmics, Planegg/Martinsried, Germany; <sup>4</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>5</sup>Biognosys AG, Zuerich, Switzerland; <sup>6</sup>Bruker S.R.O., Brno, Czech Republic
- TP 330 **Mass spectrometry-based proteomics is an orthogonal methodology to affinity-based technology;** Ann-Christine König<sup>1</sup>; Thomas Gronauer<sup>1</sup>; Andreas Schmidt<sup>2</sup>; Marcel Blindert<sup>1</sup>; Fabian Gruhn<sup>1</sup>; Zuzana Demianova<sup>3</sup>; Juliane Merl-Pham<sup>1</sup>; Stefanie Hauck<sup>1</sup>; <sup>1</sup>Helmholtz Munich, Munich, Germany; <sup>2</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>3</sup>PreOmics GmbH, München, Germany
- TP 331 **Introducing novel high-capacity and easy-to-use Empore membrane-based methods for proteome and**

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- metabolome analysis; Gregory A Davidson<sup>1</sup>; Yanbao Yu<sup>1,2</sup>; Guotao Lu<sup>1</sup>; Xiaohui Zhang<sup>1</sup>; <sup>1</sup>CDS Analytical LLC, Oxford, PA; <sup>2</sup>University of Delaware, Newark, DE
- TP 332 **Characterizing Trypsin Proteoforms and Their Impact on Digestion Efficiency and Specificity**; Shailin Patel<sup>1</sup>; Victoria C. Cotham<sup>1</sup>; Shunhai Wang<sup>1</sup>; Ning Li<sup>1</sup>; <sup>1</sup>Regeneron Pharmaceuticals, Tarrytown, NY
- TP 333 **A novel on-filter in-cell digestion (OFIC) approach enables rapid and in-depth proteome profiling of lintact cells with minimal input**; Yanbao Yu<sup>1</sup>; Jessica L Keffer<sup>1</sup>; Guotao Lu<sup>2</sup>; Gregory A Davidson<sup>2</sup>; <sup>1</sup>University of Delaware, Newark, DE; <sup>2</sup>CDS Analytical LLC, Oxford, PA
- TP 334 **Incorporation of hydrophilic magnetic beads into proteomic workflows**; Ellen Crummy<sup>1</sup>; Chris Hosfield<sup>1</sup>; Elizabeth Caine<sup>1</sup>; Kristin Riching<sup>1</sup>; Marjeta Urh<sup>1</sup>; Mike Rosenblatt<sup>1</sup>; <sup>1</sup>Promega Corporation, Madison, Wisconsin
- TP 335 **Proteomics analysis of limited number of cells by a rapid and efficient workflow using adaptive focused acoustic technology**; Anu Jain<sup>1</sup>; M Cristine C. Charlesworth<sup>2</sup>; Sameer Vasantgadkar<sup>3</sup>; Debadeep Bhattacharyya<sup>3</sup>; Akhilesh Pandey<sup>2</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN; <sup>2</sup>Mayo clinic, Rochester, MN; <sup>3</sup>Covaris, LLC, Woburn, MA
- TP 336 **Streamlined Proteomic Sample Preparation: On-Column Protein Digestion coupled to Automated Peptide Desalting**; Heather Eastwood<sup>1</sup>; Fabian Wendt<sup>2</sup>; Qi Huang<sup>1</sup>; John D Laycock<sup>1</sup>; <sup>1</sup>Tecan, Baldwin Park, CA; <sup>2</sup>TECAN Group, Männedorf, Switzerland
- TP 337 **Development of an LCMS method for polyamine analysis using carbonylated derivatives**; Megan R Gendjar<sup>1</sup>; Christine Isaguirre<sup>1</sup>; Ryan D Sheldon<sup>1</sup>; <sup>1</sup>Van Andel Research Institute, Grand Rapids, MI
- TP 338 **Evaluating Sample Preparation methods in a Core facility environment for samples with low amounts of protein**; Gabriela Grigorean<sup>1</sup>; Lauren Yoon Dixon<sup>1</sup>; Brett S. Phinney<sup>1</sup>; <sup>1</sup>University of California - Davis, Davis, CA
- TP 339 **Benchmarking magnetic Streptavidin beads for high-throughput enrichment of biotinylated proteins**; Vineet Vaibhav<sup>1,2</sup>; Toby Dite<sup>1,2</sup>; Jumana Yousef<sup>1,2</sup>; Ryan S Cross<sup>1,3</sup>; Alexander J Davenport<sup>1,3</sup>; Misty R Jenkins<sup>1,3</sup>; Laura F Dagley<sup>1,2</sup>; <sup>1</sup>WEHI, Parkville, Australia; <sup>2</sup>Department of Medical biology, University of Melbourne, Melbourne, Australia; <sup>3</sup>Immunology Division, The Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia
- TP 340 **Method development for the simultaneous analysis of drugs of abuse in fish tissue**; DIANA M CARDENAS SORACA<sup>1</sup>; Paola A. Ortiz-Suarez<sup>2</sup>; Sandra Salic<sup>2</sup>; Rashne Vakharia<sup>2</sup>; Leslie M. Bragg<sup>2</sup>; Mark R. Servos<sup>2</sup>; <sup>1</sup>UNIVERSITY OF WATERLOO, Waterloo, ON; <sup>2</sup>University of Waterloo, Waterloo, ON
- TP 341 **Solid Phase Extraction Of Fentanyl Analogs And Xylazine In Urine Using HPSCX Columns On The Resolvex® i300/A200 Instruments**; Heather Eastwood<sup>1</sup>; Steven Alo<sup>1</sup>; Qi Huang<sup>1</sup>; Karsten Liegmann<sup>1</sup>; John D Laycock<sup>1</sup>; <sup>1</sup>Tecan, Baldwin Park, CA
- TP 342 **Rapid, Semi-automated Enzyme Profiling**; Jolene K Diedrich<sup>1,2</sup>; Antonio F. M. Pinto<sup>2</sup>; Casimir Bamberger<sup>1</sup>; John R. Yates III<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>Salk Institute for Biological Studies, La Jolla, CA
- TP 343 **High throughput proteomics analyses of Immunoglobulin bound and circulating free proteins in human plasma**; Huiling Liu<sup>1</sup>; Hiroyuki Katayama<sup>1</sup>; Yining Cai<sup>1</sup>; Johannes Francois Fahrman<sup>1</sup>; Jody Vykoukal<sup>1</sup>; Matthew Willetts<sup>1</sup>; Diego Assis<sup>2</sup>; Elizabeth Gordon<sup>2</sup>; Samir Hanash<sup>1</sup>; <sup>1</sup>Department of Clinical Cancer Prevention, The University of Texas MD Anderson Cancer Center, Houston, TX; <sup>2</sup>Bruker Scientific LLC, Billerica, MA
- TP 344 **Navigating the inherent challenges with dilute and shoot: an investigation using protein depletion plates**; Lauren E Seveney; <sup>1</sup>Dominion Diagnostics, LLC, North Kingstown, RI
- TP 345 **Benchmarking a low-cost automated sample preparation platform for highly multiplexed blood plasma proteomics**; Eric F. Zaniewski<sup>1,2</sup>; Benedikt C. Clemens<sup>1,2</sup>; Robert Morris<sup>1,2</sup>; Johannes Kreuzer<sup>1,2</sup>; Soroush Hajizadeh<sup>1,2</sup>; Marc S. Weinberg<sup>1,2</sup>; Mahesh Chandra Kodali<sup>1,2</sup>; Pia Kivisakk<sup>1,2</sup>; Steven E. Arnold<sup>1,2</sup>; Wilhelm Haas<sup>1,2</sup>; <sup>1</sup>Massachusetts General Hospital (MGH), Charlestown, MA; <sup>2</sup>Harvard Medical School, Boston, MA
- TP 346 **Optimized instrument configuration for the Orbitrap Astral mass spectrometer in data-dependent acquisition (DDA) and data-independent acquisition (DIA) modes**; Ivo A Hendriks<sup>1</sup>; Sara C. Buch-Larsen<sup>1</sup>; Martin Rykær<sup>1</sup>; Michael L Nielsen<sup>1</sup>; <sup>1</sup>Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, København, Denmark

### LIPIDS: GENERAL 347-378

- TP 347 **Bi-Modal Fluorescence-Mass Spectrometry for Lipid Characterization**; Dallas Freitas<sup>1</sup>; Gopal Reddy<sup>1</sup>; Xin Yan<sup>1</sup>; <sup>1</sup>Texas A&M, College Station, TX
- TP 348 **Building a Multidimensional Oxylipin Library Containing Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry Information**; Amie M. Solosky<sup>1</sup>; Olivier Salamin<sup>2</sup>; Jack P. Ryan<sup>1</sup>; James N. Dodds<sup>1</sup>; Craig E. Wheelock<sup>2,3</sup>; Erin S. Baker<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>2</sup>Karolinska Institutet, Stockholm, Sweden; <sup>3</sup>Karolinska University Hospital, Stockholm, Sweden
- TP 349 **Comparing Storage Conditions for the Analysis of Extracted Lipids from Latent Fingerprints: Liquid Extracts vs Frozen Foils**; Aleesa E Chua<sup>1</sup>; Eden P. Go<sup>1</sup>; Heather Desaire<sup>1</sup>; <sup>1</sup>University of Kansas, Lawrence, KS
- TP 350 **Kinetic isotopic tracing unravels the de novo synthesis and metabolism of phospholipid isomers at C=C location level**; Zhuoning Xie<sup>1</sup>; Zheng Ouyang<sup>1</sup>; Xiaoxiao Ma<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China
- TP 351 **Lipid labeling method to identify alternative carbon sources during glucose starvation**; Rebekah L Mokry<sup>1,2</sup>; John G Purdy<sup>1,2,3</sup>; <sup>1</sup>BIO5 Institute, University of Arizona, Tucson, AZ; <sup>2</sup>Department of Immunobiology, University of Arizona, Tucson, AZ; <sup>3</sup>Cancer Biology Interdisciplinary Program, University of Arizona, Tucson, AZ
- TP 352 **Formation of iron adduct ions of some Polyunsaturated fatty acids under ESI conditions: Potential suppression of overall LC-MS sensitivity**; Josef Ruzicka<sup>1</sup>; France Landry<sup>1</sup>; Petia Shipkova<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb, Lawrenceville, NJ
- TP 353 **Analysis of Enterococcus faecalis Glycerophospholipids and Fatty Acid Incorporation by Ion Mobility-Mass Spectrometry and Paternò-Büchi C=C Analysis**; Rebekah L Phelan<sup>1</sup>; Hannah M Hynds<sup>1</sup>; Kelly M Hines<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- TP 354 **Stability Study of mRNA- Lipid Nanoparticles under Different Formulation and Storage Conditions**; David Wong<sup>1</sup>; Suresh Babu Cv<sup>2</sup>; Ravindra Gudihal<sup>2</sup>; Li Zhang<sup>3</sup>; Yi Yan Yang<sup>3</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Agilent Technologies Singapore (sales) Pte Ltd, Singapore, Singapore; <sup>3</sup>Bioprocessing Technology Institute, Agency for Science, Technology and Research, Singapore, Singapore
- TP 355 **Analysis of Lipid Nanoparticle Components by MALDI Trapped Ion Mobility Spectrometry**; Sergei Dikler; <sup>1</sup>Bruker Scientific, LLC, Billerica, MA
- TP 356 **Analysis of Tissue Lipid Incorporation by Staphylococcus aureus**; David T Brewer<sup>1</sup>; Kelly M. Hines<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- TP 357 **Fast Lipid Analysis of Lipid A Coupled with Tandem Mass Spectrometry**; Katelynn S. Zuercher<sup>1</sup>; Erin H. Seeley<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>University of Texas at Austin, Austin, TX
- TP 358 **Gordonia amarae and Mycobacterium tuberculosis mycolic acid isomers revealed by cyclic ion mobility (cIM)-mass spectrometry (MS)**; Hector De Las Heras Prieto<sup>1</sup>; Rachel Schwartz-Narbonne<sup>1</sup>; Laura Cole<sup>1</sup>; Martin Palmer<sup>2</sup>; Sarah Forbes<sup>1</sup>; <sup>1</sup>Sheffield Hallam University,

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- Sheffield, United Kingdom; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom
- TP 359 **Characterization of Complex Cardiolipins by Liquid Chromatography with Hybrid CID and UVPD;** Olivia E Dioli<sup>1</sup>; Melanie J Campbell<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>University of Texas at Austin, Austin, Texas
- TP 360 **Phosphatidylethanol Signatures in Blood May Help Determine Patterns of Alcohol Consumption;** Sangeeta Pandey<sup>1</sup>; Harmeet Kaur Chohan<sup>1</sup>; Peter L. Anderson<sup>2</sup>; Kristina M. Brooks<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, Department of Chemistry, West Lafayette, IN; <sup>2</sup>University of Colorado, Anschutz Medical Campus, Department of Pharmaceutical Sciences, Aurora, CO
- TP 361 **Minimizing Lipid Fragmentation Utilizing HPLC-Ultrasonic Nebulization-Corona Discharge Ionization Mass Spectrometry (HPLC-USN-CD-MS);** Qian Ma<sup>1</sup>; Theresa Evans-Nguyen<sup>1</sup>; <sup>1</sup>University of South Florida, Tampa, FL
- TP 362 **Untargeted LC-MS characterization of human breast tumor cell lines reveals subtype-specific differences in the lipidome;** William D. Gwynne<sup>1</sup>; Nicholas S. Ly<sup>1</sup>; Jeremy K. Chan<sup>1</sup>; Brandon Y. Lieng<sup>1</sup>; Olivia Taverniti<sup>1</sup>; Andrew T. Quaille<sup>1</sup>; J. Rafael Montenegro-Burke<sup>1</sup>; <sup>1</sup>Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON
- TP 363 **Unlocking E. Coli's lipidomes: delving into the dynamic composition of different strains;** Amy K Wycislik<sup>1</sup>; Adriana Zardini Buzatto<sup>1, 2</sup>; <sup>1</sup>University of Calgary, Calgary, AB; <sup>2</sup>Calgary Metabolomics Research Facility, Calgary, AB
- TP 364 **Optimization of a micro-LC-MS/MS method for untargeted Lipidomics;** Fernanda Sousa Monteiro<sup>1</sup>; Liang Li<sup>1, 2</sup>; <sup>1</sup>University of Alberta, Edmonton, AB; <sup>2</sup>The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta
- TP 365 **Lipidomics reveals altered hepatic lipid metabolism in response to acetaminophen overdose;** Ahsan Hameed<sup>1, 2</sup>; Colin D. Kay<sup>3</sup>; Mario G. Ferruzzi<sup>3</sup>; Andrew J Morris<sup>3, 4, 5</sup>; Mitchell McGill<sup>6</sup>; <sup>1</sup>Arkansas Children's Nutrition Center, Little Rock, AR; <sup>2</sup>Department of Pediatrics, University of Arkansas for Medical Sciences, Little Rock, AR; <sup>3</sup>Arkansas Children's Nutrition Center, University of Arkansas for Medical Sciences, Little Rock, AR; <sup>4</sup>Department of Pharmacology and Toxicology, University of Arkansas for Medical Sciences, Little Rock, AR; <sup>5</sup>Central Arkansas Veterans Affairs Healthcare System, Little Rock, AR; <sup>6</sup>Department of Environmental Health Sciences, Fay W. Boozman College of Public Health, University of Arkansas for Medical Sciences, Little Rock, AR
- TP 366 **Lipids as Indicators of Successful Fecal Microbiota Transplantations;** Guozhi Zhang<sup>1</sup>; Arthur S. McMillan<sup>2</sup>; Jessie R. Chapel<sup>2</sup>; Casey M. Theriot<sup>2</sup>; Erin S. Baker<sup>1</sup>; <sup>1</sup>UNC-Chapel Hill, Chapel Hill, NC; <sup>2</sup>North Carolina State University, Raleigh, NC
- TP 367 **Lipidomics of NASH human liver organoids align with liver biopsies of NASH patients;** Nate F Schmidt<sup>1</sup>; Ekta Minocha<sup>1</sup>; Ashwani Gupta<sup>1</sup>; Jason Wertheim<sup>1</sup>; Richard Green<sup>2</sup>; John G Purdy<sup>1</sup>; <sup>1</sup>BIO5 Institute, University of Arizona, Tucson, AZ; <sup>2</sup>Northwestern University Feinberg School of Medicine, Chicago, IL
- TP 368 **Investigating the Role of Circulating small extracellular vesicles Lipids in Prostate Cancer;** Marco Ghirimoldi<sup>1</sup>; Marco Falasca<sup>2</sup>; Marcello Manfredi<sup>3</sup>; Elettra Barberis<sup>4</sup>; <sup>1</sup>University of Piemonte Orientale, Novara, Italy; <sup>2</sup>Università di Parma, Parma, Italy; <sup>3</sup>DIMET, Novara, Italy; <sup>4</sup>DISIT, Alessandria, Italy
- TP 369 **Probing the Environmental Fortitude of mRNA Lipid Nanoparticles: A TIMS-TOF Insights into Stress-Induced Degradation;** Michael Girgis<sup>1</sup>; Beixi Wang<sup>2</sup>; Xuejun Peng<sup>2</sup>; Hooda Said<sup>1</sup>; Suman Alishetty<sup>1</sup>; Manuel Carrasco<sup>1</sup>; Dillon O'Neill<sup>1</sup>; Nabilah Baby<sup>1</sup>; Gregory Petruncio<sup>1</sup>; Mohamad-Gabriel Alameh<sup>3</sup>; Caroline Hoemann<sup>1</sup>; Matthew Albano<sup>4</sup>; Erica Marie Forsberg<sup>2</sup>; Mikell Paige<sup>1</sup>; <sup>1</sup>George Mason University, Manassas, VA; <sup>2</sup>Bruker Scientific LLC, San Jose, CA; <sup>3</sup>University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; <sup>4</sup>Bruker Scientific, LLC, Billerica, MA
- TP 370 **One-Step Lipid Mass Tags for Probing Unsaturated Lipid Isomers and Accurate Relative Quantification;** Gopal Reddy Ramidi<sup>1</sup>; Tingyuan Yang<sup>1</sup>; Xin Yan<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX
- TP 371 **Employing vacuum jacketed columns and prototype benchtop multi reflecting time-of-flight (MRT) to increase lipidomic throughput whilst maintaining highly confident identifications;** Matthew E Daly<sup>1</sup>; Nyasha Munjoma<sup>1</sup>; Robert S Plumb<sup>2</sup>; Jason Hill<sup>2</sup>; Nick Tomczyk<sup>1</sup>; Lee A Gethings<sup>1</sup>; Richard Lock<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Waters Corporation, Milford, MA
- TP 372 **Complex Lipid Mixture Analysis using Homemade SPE-ESI-MS;** Octavio Spears<sup>1</sup>; Alex Grooms<sup>2</sup>; Benjamin Burris<sup>2</sup>; Abraham K. Badu-Tawiah<sup>2</sup>; <sup>1</sup>The Ohio State University, Columbus, OH; <sup>2</sup>Ohio State University, Columbus, OH
- TP 373 **Impact of Contaminants from Plasticware Used in Sample Preparation on Human Serum Lipidome Analysis;** Carlos R. Canez<sup>1</sup>; Liang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, AB
- TP 374 **nano-lipidomics employing silica based monolithic columns;** Matthias Schittmayer-Schantl<sup>1</sup>; Goran Mitulovic<sup>2</sup>; Michael Krawitzky<sup>2</sup>; Gary Kruppa<sup>3</sup>; Ruth Birner-Gruenberger<sup>1</sup>; <sup>1</sup>TU Wien, Vienna, Austria; <sup>2</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>3</sup>Bruker S.R.O., Brno, Czech Republic
- TP 375 **Assessing changes in sebum lipids according to anatomical collection region and biological sex;** Madeline Isom<sup>1</sup>; Eden P. Go<sup>1</sup>; Heather Desaire<sup>1</sup>; <sup>1</sup>The University of Kansas, Lawrence, KS
- TP 376 **Monitoring the Exchange of Cholesterol Between Nanodiscs by APCI;** Annika Silverberg<sup>1</sup>; Michael Marty<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ
- TP 377 **Using data-dependent and independent hybrid acquisitions for fast liquid chromatography-based untargeted lipidomics;** Kanako Tokiyoshi<sup>1</sup>; Yuki Matsuzawa<sup>1</sup>; Mikiko Takahashi<sup>2</sup>; Hiroaki Takeda<sup>1, 3</sup>; Kozo Nishida<sup>4</sup>; Mayu Hasegawa<sup>4</sup>; Junki Miyamoto<sup>4</sup>; Hiroshi Tsugawa<sup>1, 2, 3, 5, 6</sup>; <sup>1</sup>Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology, Koganei-shi, Japan; <sup>2</sup>RIKEN Center for Sustainable Resource Science, Yokohama, Japan; <sup>3</sup>RIKEN Center for Brain Science, Wako, Japan; <sup>4</sup>Department of Applied Biological Science, Tokyo University of Agriculture and Technology, Fuchu, Japan; <sup>5</sup>RIKEN Center for Integrative Medical Sciences, Yokohama, Japan; <sup>6</sup>Molecular and Cellular Epigenetics Laboratory, Graduate School of Medical Life Science, Yokohama City University, Yokohama, Japan
- TP 378 **Resolving Method Development Challenges in the Assay Validation of PEG-Lipid Quantitation;** Melissa Roberts<sup>1</sup>; Ryan Lo<sup>1</sup>; Ling Morgan<sup>1</sup>; <sup>1</sup>Moderna, Cambridge, MA

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- TP 379 **Localization of lipid C=C bond positions using nitroarenes via photoirradiation and mass spectrometry;** Xi Chen<sup>1</sup>; Gopal Reddy Ramidi<sup>1</sup>; Annesha Sengupta<sup>1</sup>; Luchen Wuyang<sup>1</sup>; Aidan Slagter<sup>1</sup>; Nitya Shree<sup>2</sup>; Mahua Choudhury<sup>2</sup>; Xin Yan<sup>1</sup>; <sup>1</sup>Department of Chemistry, Texas A&M University, College Station, TX; <sup>2</sup>Department of Pharmaceutical Sciences, Texas A&M University, College Station, TX
- TP 380 **Chemical Conjugation Method for Enhanced Diacylglycerol Multiple Reaction Monitoring Profiling;** Harshit Arora<sup>1</sup>; Pooja Saklani<sup>2</sup>; Guang Yang<sup>2</sup>; Caitlin Randolph<sup>3</sup>; Gaurav Chopra<sup>2, 4, 5, 6, 7, 8</sup>; <sup>1</sup>PURDUE UNIVERSITY, West Lafayette, IN; <sup>2</sup>Purdue University, Department of Chemistry, West Lafayette, IN; <sup>3</sup>Purdue University Department of Chemistry, West Lafayette, IN; <sup>4</sup>Purdue Institute for Drug Discovery, West Lafayette, IN; <sup>5</sup>Purdue Institute for Cancer Research, Purdue University,



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- West Lafayette, IN; <sup>6</sup>Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; <sup>7</sup>Purdue Institute for Integrative Neuroscience, West Lafayette, IN; <sup>8</sup>Purdue University, Department of Computer Science, West Lafayette, IN
- TP 381 **Analysis of novel Caenorhabditis elegans-specific phosphorylated sphingolipids using LC-TIMS-MS/MS and MassQL**; Michael Witting<sup>1,2</sup>; Liesa Salzer<sup>3</sup>; Sven Myer<sup>4</sup>; Aiko Barsch<sup>4</sup>; Russell Waugh<sup>5</sup>; <sup>1</sup>Metabolomics and Proteomics Core, Helmholtz Zentrum München German Research Center for Environmental Health, Neuherberg, Germany; <sup>2</sup>Chair of Analytical Food Chemistry, TUM School of Life Sciences, Technical University of Munich, Freising-Weiherstephan, Germany; <sup>3</sup>Research Unit Analytical BioGeoChemistry, Helmholtz Zentrum München German Research Center for Environmental Health, Neuherberg, Germany; <sup>4</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitsstraße 4, 28359 Bremen, Germany; <sup>5</sup>Bruker Scientific LLC, Denver, CO
- TP 382 **Photochemical Tissue Pre-processing for Matrix-Assisted Laser Desorption Ionization Imaging of Lipids**; Taylor Bell<sup>1</sup>; Kadeem O Hayes<sup>1</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA
- TP 383 **Multidimensional Characterization of Oxidized Lipids Using HILIC - Ion Mobility - Mass Spectrometry**; Noelle Reimers<sup>1</sup>; Libin Xu<sup>2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA
- TP 384 **Novel Ion Fragmentation for Detailed Lipid Structural Analysis via Atomic Hydrogen/Oxygen Irradiation (HAD/OAD)**; Hidenori Takahashi<sup>1</sup>; Yohei Arao<sup>1</sup>; Kaoru Nakagawa<sup>1</sup>; Yuta Miyazaki<sup>1</sup>; Takanari Hattori<sup>1</sup>; Natsuyo Asano<sup>1</sup>; <sup>1</sup>Shimadzu, Kyoto, Japan
- TP 385 **Charge switching isomeric and isobaric lipid cations for chemical separation with subsequent carbon-carbon double bond localization**; Kimberly C. Fabijanczuk<sup>1</sup>; Boukar K. S. Faye<sup>1</sup>; Catilin E. Randolph<sup>1</sup>; Scott A. McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, Department of Chemistry, West Lafayette, IN
- TP 386 **Charge Switching OzESI-MRM Strategy for Isomer-Specific Fatty Acid Profiling of Lipid Droplets with Relation to Alzheimer's Disease and Aging**; Caitlin Randolph<sup>1</sup>; Palak Manchanda<sup>1</sup>; Sanjay Iyer<sup>1</sup>; Shane Tichy<sup>2</sup>; Gaurav Chopra<sup>1,3,4,5,6,7</sup>; <sup>1</sup>Purdue University, Department of Chemistry, West Lafayette, IN; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>Purdue Institute for Integrative Neuroscience, West Lafayette, IN; <sup>4</sup>Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; <sup>5</sup>Purdue University, Department of Computer Science, West Lafayette, IN; <sup>6</sup>Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; <sup>7</sup>Purdue Institute for Drug Discovery, West Lafayette, IN
- TP 387 **High Resolution Ion Mobility Incorporating Traveling Wave Structures for Lossless Ion Manipulation Unveils Hidden Lipid Features within Total Lipid Fractions**; Allison R Reardon<sup>1</sup>; Katrina L Leaptrot<sup>1</sup>; Jody C May<sup>1</sup>; John A McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN
- TP 388 **Spatial mapping of phosphatidylcholine sn-position isomers using CID of divalent metal complexes in imaging mass spectrometry**; Tingting Yan<sup>1</sup>; Zunaira Naeem<sup>1</sup>; Boone M. Prentice<sup>1</sup>; <sup>1</sup>The University of Florida, Gainesville, FL
- TP 389 **Lipid A double bond position determination using ozone and laser-induced dissociation**; ABANOUB MIKHAEL<sup>1,2</sup>; HELENA PETROSOVA<sup>1,2</sup>; DEREK SMITH<sup>2</sup>; ROBERT K ERNST<sup>3</sup>; DAVID R GOODLETT<sup>1,2</sup>; <sup>1</sup>University of Victoria, Victoria, BC; <sup>2</sup>University of Victoria Genome BC Proteomic Centre, Victoria, British Columbia; <sup>3</sup>University of Maryland, Baltimore, Baltimore, MD
- TP 390 **Resolving the Geometry and Location of Lipid Unsaturation by Radical-Induced Isomerization and RPLC-MS/MS Coupled with Online Paternò-Büchi Reaction**; Hengxue Shi<sup>1</sup>; Yu Xia<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China
- TP 391 **Deep profiling of phosphoinositide phosphates from cells and organelles**; Zidan Wang<sup>1</sup>; Xue Jin<sup>1</sup>; Hanlin Ren<sup>2</sup>; Shuaiting Yan<sup>1</sup>; Hang Yin<sup>1</sup>; Yu Xia<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>The University of Texas at Austin, Austin, TX
- TP 392 **Identification and quantitation of impurities of the ionizable lipid ALC-0315 for vendor-to-vendor raw material assessment to ensure mRNA-LNP product quality**; Todd Stawicki<sup>1</sup>; Mays Al-Dulaymi<sup>2</sup>; Zhichang Yang<sup>3</sup>; Sahana Mollah<sup>4</sup>; Jonathan Le Huray<sup>2</sup>; Roxana McCloskey<sup>1</sup>; <sup>1</sup>Sciex, Framingham, MA; <sup>2</sup>Acuitas Therapeutics Inc., Vancouver, BC; <sup>3</sup>Genentech, Inc., South San Francisco, CA; <sup>4</sup>SCIEX, Redwood City, CA
- TP 393 **Deep profiling of gut bacteria lipidome via data-dependent acquisition and radical-directed dissociation-tandem mass spectrometry**; Ruijun Jian<sup>1</sup>; Xiaoyi Zhu<sup>2</sup>; Hailiang Liu<sup>2</sup>; Yu Xia<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>State Key Laboratory of Cardiology and Medical Innovation Center, Shanghai East Hospital, School of Medicine, Tongji University, Shanghai, China
- TP 394 **Characterizing Lipid Isomers Using Superior Ion Mobility Separations and Ultrafast Ozone-Induced Dissociation of Multiply Charged Transition Metal Complexes**; Alexandre A Shvartsburg<sup>1</sup>; Hayden A Thurman<sup>1</sup>; Pawel Sadowski<sup>2</sup>; Berwyck LJ Poad<sup>2</sup>; Stephen J Blanksby<sup>2</sup>; <sup>1</sup>Wichita State University, Wichita, KS; <sup>2</sup>Queensland University of Technology, Brisbane, Australia
- TP 395 **Oxygen Attachment Dissociation (OAD) MS/MS for the structural identification of double-bond positions in different lipid classes associated with alcohol toxicity**; Emily G Armitage<sup>1</sup>; Paolo Redegalli<sup>2</sup>; Alan Barnes<sup>1</sup>; Olga Dedea<sup>3</sup>; Thomas Meikopoulos<sup>3</sup>; Christina Virgiliou<sup>3</sup>; Helen Gika<sup>3</sup>; Neil J Loftus<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Manchester, United Kingdom; <sup>2</sup>Shimadzu Italia S.r.l., Milano, Italy; <sup>3</sup>BIOMIC\_AUTH, CIRI, Aristotle University of Thessaloniki, Thessaloniki, Greece
- TP 396 **Investigating Structural Lipidomic Alterations in Subjects Positive for Illicit Drugs with SFC-APPI-CID of Electron-Deficient Precursors and SFC-ESI-CID/EAD**; Patrick Mueller<sup>1</sup>; Stefan König<sup>2</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>University of Geneva, Geneva, Switzerland; <sup>2</sup>University of Bern, Bern, Switzerland
- TP 397 **Empirically determined adduct ratios and in-source fragments enhance lipid species identification**; Nicholas S Ly<sup>1</sup>; Jeremy K Chan<sup>1</sup>; William D Gwynne<sup>1</sup>; Brandon Y Lieng<sup>1</sup>; Andrew T Quaille<sup>1</sup>; Cunjie Zhang<sup>1</sup>; J. Rafael Montenegro-Burke<sup>1</sup>; <sup>1</sup>Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON
- METABOLOMICS: CLINICAL APPLICATIONS**  
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- TP 398 **Neonatal Metabolomics: The Untold Stories in Infant's Blood**; Carter Asef<sup>1</sup>; Samuel G. Moore<sup>1</sup>; C. Austin Pickens<sup>2</sup>; Carlos A. Saavedra-Matiz<sup>3</sup>; Joseph J. Orsini<sup>3</sup>; Konstantinos Petritis<sup>2</sup>; David A. Gaul<sup>1</sup>; Facundo M. Fernandez<sup>1,4</sup>; <sup>1</sup>School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Division of Laboratory Sciences, National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, GA; <sup>3</sup>Newborn Screening Program, Wadsworth Center, New York State Department of Health, Albany, NY; <sup>4</sup>Petit Institute of Biengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA
- TP 399 **Identification of urine metabolic biomarkers for diagnosing membranous nephropathy and its subtype**; Yufei Li<sup>1</sup>; Ji Hye Kim<sup>2</sup>; Jihyun Kang<sup>1,3</sup>; Seung Seok Han<sup>4</sup>; Joo-Youn Cho<sup>1,5</sup>; <sup>1</sup>Department of Clinical Pharmacology and Therapeutics, Seoul National University College of Medicine and Hospital, Seoul, South Korea; <sup>2</sup>Department of Internal Medicine, Chungbuk National University Hospital, Seoul, South Korea; <sup>3</sup>Kidney Research Institute, Seoul National University Medical Research Center, Seoul, South Korea;

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- <sup>4</sup>Department of Internal Medicine, Seoul National University College of Medicine, Seoul, South Korea; <sup>5</sup>Department of Biomedical Sciences, Seoul National University College of Medicine, Seoul, South Korea
- TP 400 **Metabolomic Profiling Reveals Alterations in Arginine Biosynthesis Induced by  $\beta$ -Lapachone Derivative;** YEONSEO JANG<sup>1</sup>; Jihyun Kang<sup>1,2</sup>; Yufei Li<sup>1</sup>; Eunsol Yang<sup>1,3</sup>; SeungHwan Lee<sup>1</sup>; Joo-Youn Cho<sup>1,4</sup>; <sup>1</sup>Department of Clinical Pharmacology and Therapeutics, Seoul National University College of Medicine and Hospital, Seoul, South Korea; <sup>2</sup>Kidney Research Institute, Seoul National University Medical Research Center, Seoul, South Korea; <sup>3</sup>Department of Bioengineering and Therapeutic Sciences, University of California, San Francisco, San Francisco, CA; <sup>4</sup>Department of Biomedical Sciences, Seoul National University College of Medicine, Seoul, South Korea
- TP 401 **Screening of organic acids for nutritional and metabolic profiling from dried urine spots using Gas Chromatograph Mass Spectrometer;** Aseem Rajan Wagle<sup>1</sup>; Prashant Hase<sup>1</sup>; Bhaumik Trivedi<sup>1</sup>; Sanket Chiplunkar<sup>1</sup>; Durvesh Sawant<sup>1</sup>; Rahul Dwivedi<sup>1</sup>; Hemant Kesarkar<sup>1</sup>; Mohit Sharma<sup>1</sup>; Satyendra Singh<sup>1</sup>; Pratap Rasam<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; <sup>1</sup>Shimadzu Analytical India Pvt. Ltd., Mumbai, India
- TP 402 **Untargeted metabolomic and lipidomic analyses reveal renal complications in COVID-19: molecular insights from a pilot study;** Patrick Ferreira<sup>1</sup>; Lucia Andrade<sup>2</sup>; Alessandra Sussulini<sup>1,3</sup>; <sup>1</sup>Laboratory of Bioanalytics and Integrated Omics (LaBIOmics), University of Campinas (UNICAMP), Campinas, Brazil; <sup>2</sup>Basic Research Laboratory in Renal Diseases, Faculty of Medicine, University of São Paulo (USP), São Paulo, Brazil; <sup>3</sup>National Institute of Science and Technology of Bioanalytics (INCTBio), University of Campinas (UNICAMP), Campinas, Brazil
- TP 403 **Diagnostic Biomarker Discovery Platform for Malignant Pancreatic Cysts by LC-HR-MS with Targeted and Untargeted Data Analysis;** Li Zhang<sup>1</sup>; Hong Sun Kim<sup>2</sup>; Harrison Wong<sup>3</sup>; Costas A Lyssiotis<sup>3</sup>; Jiaqi Shi<sup>2</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Department of Pathology, University of Michigan, Ann Arbor, Michigan 48109, United States, Ann Arbor, Michigan; <sup>3</sup>University of Michigan, Medical School, Ann Arbor, Michigan
- TP 404 **Establishing a high throughput LC-MS based metabolomics study for the deep phenotyping of plasma sample from cohorts investigating heart failure;** Fabian Schmitt<sup>1</sup>; Thierry Schmidlin<sup>1</sup>; <sup>1</sup>Institute of Immunology, University Medical Center of the Johannes-Gutenberg University, Mainz, Germany
- TP 405 **Antidepressant screening via Andrew+ sample preparation automation and LC-MS/MS to access microbiota and drug interactions;** Charlotte Hemmila<sup>1</sup>; Christopher Basting<sup>2</sup>; Sophia Lebakken<sup>2</sup>; Melisa Bailey<sup>2</sup>; Erik Swanson<sup>2</sup>; Courtney Broedlow<sup>2</sup>; Tim Griffin<sup>1</sup>; Emily M Cherenack<sup>3</sup>; Nichole R Klatt<sup>2</sup>; Candace Guerrero<sup>1,2</sup>; <sup>1</sup>University of Minnesota, Center for Metabolomics and Proteomics, Minneapolis, MN; <sup>2</sup>University of Minnesota, Department of Surgery, Division of Surgical Outcomes and Precision Medicine Research, Minneapolis, MN; <sup>3</sup>University of Miami, Miller School of Medicine, Department of Psychiatry and Behavioral Sciences, Miami, FL
- TP 406 **Supraphysiological vitamin C dosing in cancer patients and healthy controls reveals products of oxidative stress in the catabolism of heme;** Philenroza Thavrin<sup>1,2,3</sup>; Jaewoo Choi<sup>2</sup>; Ping Chen<sup>4</sup>; Paige Jamieson<sup>2,5</sup>; Qi Chen<sup>4</sup>; Jeanne Drisko<sup>6</sup>; Jan F. Stevens<sup>2,3</sup>; <sup>1</sup>College of Science, Oregon State University, Corvallis, OR; <sup>2</sup>Linus Pauling Institute, Oregon State University, Corvallis, OR; <sup>3</sup>College of Pharmacy, Oregon State University, Corvallis, OR; <sup>4</sup>Department of Pharmacology, Toxicology & Therapeutics, University of Kansas Medical Center, Kansas City, KS; <sup>5</sup>College of Health, Oregon State University, Corvallis, OR; <sup>6</sup>Department of Internal Medicine, Integrative Medicine Research, University of Kansas Medical Center, Kansas City, KS
- TP 407 **Investigating the post-prandial metabolome under different food intake conditions with semi-targeted LC-MS/MS;** Jiangwen Dong<sup>1,2</sup>; Yi Ning Yong<sup>3</sup>; Leroy Pakkiri<sup>1,2</sup>; Gloria Leung<sup>4</sup>; Christiani Jeyakumar Henry<sup>3,5</sup>; Sumanto Haldar<sup>3</sup>; Maxine Bonham<sup>4</sup>; Chester Lee Drum<sup>1,2</sup>; <sup>1</sup>Cardiovascular Research Institute (CVRI), National University Health System (NUHS), Singapore, Singapore; <sup>2</sup>Department of Medicine, Yong Loo Lin School of Medicine, National University of Singapore (NUS), Singapore, Singapore; <sup>3</sup>Clinical Nutrition Research Centre (CNRC), Singapore Institute of Food and Biotechnology Innovation (SIFBI), Agency for Science, Technology and Research (A\*STAR), Singapore, Singapore; <sup>4</sup>Department of Nutrition, Dietetics and Food, Monash University, Melbourne, Australia; <sup>5</sup>Department of Biochemistry, National University of Singapore (NUS), Singapore, Singapore
- TP 408 **Olaris Global Panel (OGP): A highly accurate and reproducible triple quadrupole mass spectrometry-based metabolomics method for clinical biomarker discovery;** Masoumeh Dorrani<sup>1</sup>; Jifang Zhao<sup>1</sup>; Nihel Bekhti<sup>1</sup>; Alessia Trimigno<sup>1</sup>; Elizabeth O'Day<sup>1</sup>; Jurre J. Kamphorst<sup>1</sup>; <sup>1</sup>Olaris, inc, Framingham, MA
- TP 409 **Development of a 96-well plate-based sample preparation method for the assessment of drug-induced liver injury (DILI) by multi-omics analysis;** Masatomo Takahashi<sup>1</sup>; Kazuki Ikeda<sup>1</sup>; Kosuke Hata<sup>1</sup>; Takeshi Bamba<sup>1</sup>; Yoshihiro Izumi<sup>1</sup>; <sup>1</sup>Medical Institute of Bioregulation, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka-shi, Japan
- TP 410 **Deep Metabolic Phenotyping of Newborn Cord Blood Reveals Maternal Fetal Interactions and Disease Risk;** Samuel M Lancaster<sup>1</sup>; Samson Mataraso<sup>1</sup>; Jonathan Reiss<sup>1</sup>; Kevin Contrepois<sup>2</sup>; Casandra Trowbridge<sup>1</sup>; Basil Michael<sup>1</sup>; Ian Simms<sup>1</sup>; Michelle Gibson<sup>1</sup>; Max Clary<sup>1</sup>; Lettie McGuire<sup>1</sup>; Frank Wong<sup>1</sup>; Ethan Canfield<sup>1</sup>; Daniel Cotter<sup>1</sup>; Tao Wang<sup>1</sup>; Yan Yang<sup>1</sup>; Ramesh Nair<sup>1</sup>; Ylaly Katherine Bianco<sup>1</sup>; Jon Bernstein<sup>1</sup>; David Stevenson<sup>1</sup>; Tina Cowan<sup>1</sup>; Nima Aghaepour<sup>1</sup>; Maya Kasowski<sup>1</sup>; Karl Sylvester<sup>1</sup>; Michael Snyder<sup>1</sup>; <sup>1</sup>Stanford University, Stanford, CA; <sup>2</sup>AstraZeneca, South San Francisco, CA
- TP 411 **Plasma Metabolomics Evaluation Reveals SARS-CoV-2 Infection Disrupts Tryptophan and Energy Pathways with Correlations to Inflammation and Renal Status;** Jinchun Sun<sup>1</sup>; Megan Peters<sup>1</sup>; Li-Rong Yu<sup>1</sup>; Vikrant Vijay<sup>1</sup>; Heather Smallwood<sup>2</sup>; Richard Beger<sup>1</sup>; <sup>1</sup>NCTR / USFDA, Jefferson, AR; <sup>2</sup>University of Tennessee Health Science Center, Memphis, TN
- TP 412 **Application of Dried Blood Spot Microsampling for High-Throughput Four-Dimensional Trapped Ion Mobility Spectrometry Lipidomics;** Jayden Lee Roberts<sup>1,2</sup>; Luke Whaley<sup>1,2,3</sup>; Nicola Gray<sup>1,2</sup>; Melvin Gay<sup>4</sup>; Xuejun Peng<sup>5</sup>; Elaine Holmes<sup>1,2,6</sup>; Julien Wist<sup>1,2,7</sup>; Jeremy K Nicholson<sup>1,2,8,9</sup>; Nathan G Lawler<sup>1,2</sup>; <sup>1</sup>Australian National Phenome Centre, Health Futures Institute, Harry Perkins Institute, Murdoch University, Murdoch, Australia; <sup>2</sup>Centre for Computational and Systems Medicine, Health Futures Institute, Harry Perkins Institute, Murdoch University, Murdoch, Australia; <sup>3</sup>Perron Institute for Neurological and Translational Sciences, Nedlands, Australia; <sup>4</sup>Bruker Pty Ltd, Preston, Australia; <sup>5</sup>Bruker Daltonics Inc., San Jose, CA; <sup>6</sup>Department of Metabolism Digestion and Reproduction, Imperial College London, London, United Kingdom; <sup>7</sup>Chemistry Department, Universidad del Valle, Melendez, Colombia; <sup>8</sup>Department of Cardiology, Fiona Stanley Hospital, Medical School, University of Western Australia, Murdoch, Australia; <sup>9</sup>Institute of Global Health Innovation, Faculty of Medicine, Imperial College, South Kensington, United Kingdom
- TP 413 **Metabolic profiling of amniotic fluid by differential isotope dansylation labeling LC-MS for application in trisomy 21 fetuses;** Yi-Ting Chen<sup>1</sup>; Ya-Ju Hsieh<sup>1</sup>; Yao-Lung Chang<sup>2</sup>; Liang Li<sup>3</sup>; Jau-Song Yu<sup>1</sup>; <sup>1</sup>Chang Gung University,

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- Taoyuan, Taiwan; <sup>2</sup>LinKou Chang Gung Memorial Hospital, Taoyuan, Taiwan; <sup>3</sup>University of Alberta, Edmonton, AB  
 TP 414 **Exploring effects of particulate matter exposure on pregnant women via urinary metabolic profiling;** Minki Shim<sup>1</sup>; Sunwha Park<sup>2</sup>; Young Ju Kim<sup>2</sup>; Dong-Kyu Lee<sup>1</sup>; <sup>1</sup>College of Pharmacy, Chung-Ang University, Seoul, South Korea; <sup>2</sup>Department of Obstetrics and Gynecology, College of Medicine, Ewha Medical Research Institute, Ewha Womans University, Seoul, South Korea
- METABOLOMICS: IDENTIFICATION OF UNKNOWN METABOLITES  
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- TP 415 **2-Homoectoine: A New Ectoine Derivative from Phyto- and Bacterioplankton Involved in Osmoadaptation;** Muhaiminatul Azizah<sup>1</sup>; Georg Pohnert<sup>1,2</sup>; <sup>1</sup>Friedrich Schiller University Jena, Jena, Germany; <sup>2</sup>Max Planck Institute for Chemical Ecology, Jena, Germany
- TP 416 **Improved Quantification of Carbonyl Sub-metabolome by LC-MS Using a Fragmentation-Controlled Multiplexed Isotopic Tag;** Xiaobo Tian<sup>1</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>University of Geneva, Geneva, Switzerland
- TP 417 **Identification of Anatoxin-a and Relevant Metabolites in Biological Matrices with High Resolution Mass Spectrometry;** Taylor J Glatte<sup>1</sup>; Mike A Mojica<sup>2</sup>; Logan C Krajewski<sup>2</sup>; Kirsten A Cottrill<sup>1</sup>; Brady R Cunningham<sup>2</sup>; Sarah R Lagon<sup>1</sup>; Brenda Ruto<sup>3</sup>; Donna Hill<sup>4</sup>; Elizabeth I Hamelin<sup>2</sup>; <sup>1</sup>Battelle Memorial Institute, Atlanta, GA; <sup>2</sup>U.S. Centers for Disease Control and Prevention, Atlanta, GA; <sup>3</sup>Oak Ridge Institute for Science and Education, Oak Ridge, TN; <sup>4</sup>U.S. Environmental Protection Agency, Research Triangle Park, NC
- TP 418 **Small Molecule Retention Time Prediction for Nanoflow Liquid Chromatography using a Novel Machine Learning Approach;** Matthew Turner<sup>1</sup>; Luke Durell<sup>1</sup>; Sean Colby<sup>1</sup>; Sydney Schwartz<sup>1</sup>; Eva Brayfindley<sup>1</sup>; Anna Hale<sup>1</sup>; Jessica Bade<sup>1</sup>; Fanny Chu<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- TP 419 **Discovering and annotating new molecules in untargeted metabolomics through structural coupling;** Shipei Xing<sup>1,2</sup>; Yasin El Abiead<sup>1,2</sup>; Abubaker Patan<sup>1</sup>; Paulo Wender Portal Gomes<sup>1,2</sup>; Simone Zuffa<sup>1,2</sup>; Helena Mannocho-Russo<sup>1,2</sup>; Ipsita Mohanty<sup>1,2</sup>; Pieter C. Dorrestein<sup>1,2</sup>; <sup>1</sup>UC San Diego, La Jolla, CA; <sup>2</sup>Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA
- TP 420 **Real-time library search (RTLs) triggered MS3 facilitates in-depth cannabinoid profile in different hemp genotypes and identification of novel cannabinoids;** Andy C.W. Lui<sup>1</sup>; Elizabeth T Anderson<sup>1</sup>; John S Ramsey<sup>2</sup>; Kevin B Hernandez<sup>3</sup>; Yong Yang<sup>2</sup>; Zachary Stansell<sup>3</sup>; Tyler Gordon<sup>3</sup>; Theodore W Thannhauser<sup>2</sup>; Sheng Zhang<sup>1</sup>; <sup>1</sup>Proteomics and Metabolomics Facility, Cornell University, Ithaca, NY; <sup>2</sup>R.W. Holley Center for Agriculture and Health, USDA-ARS, Ithaca, NY; <sup>3</sup>Plant Genetic Resources Unit, USDA-ARS, Geneva, NY
- TP 421 **Comprehensive scoring system for high-confidence lipid identification in untargeted lipidomics;** Rui Qin<sup>1</sup>; William Xu<sup>1</sup>; Adriana Zardini Buzatto<sup>2</sup>; Elvis Lo<sup>1</sup>; Shuang Zhao<sup>1</sup>; Liang Li<sup>1,3</sup>; <sup>1</sup>The Metabolomics Innovation Centre, Edmonton, AB; <sup>2</sup>University of Calgary, Calgary, AB; <sup>3</sup>University of Alberta, Edmonton, AB
- TP 422 **Forward and Reverse Cosine Similarity Scoring During Real-Time Library Search for Triggering Additional Experiments on Indole Compounds in Plant Extract;** Brandon Bills<sup>1</sup>; Michael W Christopher<sup>2</sup>; Sunandini Yedla<sup>1</sup>; Bashar Amer<sup>1</sup>; Susan S Bird<sup>3</sup>; Rahul Deshpande<sup>1</sup>; William Barshop<sup>1</sup>; Boone M. Prentice<sup>2</sup>; Timothy J. Garrett<sup>2</sup>; Vlad Zabrouskov<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>University of Florida, Department of Chemistry, Gainesville, FL; <sup>3</sup>Thermo Fisher Scientific, Remote, MS
- TP 423 **Enabling Combined Qualitative/Quantitative CE-MS Metabolomics with Migration Time Indexing, Simplified Extraction, and a Novel Discovery Feedback Loop;** J. Will Thompson<sup>1</sup>; Erin A. Redman<sup>1</sup>; Scott Mellors<sup>1</sup>; Sam Stewart<sup>2</sup>; Joshua P. Guerrette<sup>1</sup>; Christopher D. Brown<sup>2</sup>; <sup>1</sup>908 Devices Inc, Morrisville, NC; <sup>2</sup>908 Devices Inc., Boston, MA
- TP 424 **The Shin-MassBank project: Enrichment of MassBank records using human metabolome datasets;** Fumio Matsuda<sup>1</sup>; Aykiyoshi Hirayama<sup>2</sup>; Ryosuke Hayasaka<sup>2</sup>; Masatomo Takahashi<sup>3</sup>; Akiyasu C. Yoshizawa<sup>4</sup>; Kozo Nishida<sup>5</sup>; Taihei Torigoe<sup>3</sup>; Takato Kiuchi<sup>4</sup>; Yuki Matsuzawa<sup>5</sup>; Hiroshi Tsugawa<sup>5</sup>; Shujiro Okuda<sup>4</sup>; Yoshihiro Izumi<sup>3</sup>; <sup>1</sup>Osaka University, Suita, Japan; <sup>2</sup>Keio University, Tsuruoka, Japan; <sup>3</sup>Kyushu University, Fukuoka, Japan; <sup>4</sup>Niigata University, Niigata, Japan; <sup>5</sup>Tokyo University of Agriculture and Technology, Koganei-shi, Japan
- TP 425 **Characterization of Glucosinolates in Arabis sagittata Extracts using a Multi-Reflecting Q-ToF Mass Spectrometer;** Emma Marsden-Edwards<sup>1</sup>; Sabine Metzger<sup>2</sup>; Martin Palmer<sup>1</sup>; Isabel Riba<sup>1</sup>; Vera Wewer<sup>2</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>University of Cologne, Cologne, Germany
- TP 426 **Metabolic Profile of 25E-NBOH in Human Liver Microsomes, Rat Urine and Cunnighamella elegans;** Magdalena Vagnerova<sup>1,2</sup>; Monika Mrnava<sup>1</sup>; Petr Palivec<sup>1</sup>; Bronislav Jurasek<sup>1</sup>; David Sykora<sup>2</sup>; Martin Kuchar<sup>1</sup>; <sup>1</sup>Forensic Laboratory of Biologically Active Substances, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic; <sup>2</sup>Department of Analytical Chemistry, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic
- TP 427 **Advanced Mass Spectrometry Workflows for Novel Fragmentation Approaches for Small Molecule Agrochemical Applications;** Chris J Brown<sup>1</sup>; J.C. Yves LeBlanc<sup>2</sup>; Mircea Guna<sup>2</sup>; Yelena Adelfinskaya<sup>3</sup>; Jesse Balcer<sup>3</sup>; Jeffrey R Gilbert<sup>3</sup>; <sup>1</sup>Corteva Agrisciences, Indianapolis, IN; <sup>2</sup>SCIEX, Concord, ON; <sup>3</sup>Corteva Agriscience, Indianapolis, IN
- METABOLOMICS: SAMPLE PREPARATION  
 428-437
- TP 428 **Salt Concentration in Sample Preparation has Variable Effects on Polar Feature Detection in Non-Targeted LC-MS Experiments;** David A Gaul<sup>1</sup>; Ying Liu<sup>1</sup>; Samuel G Moore<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA
- TP 429 **SWipe: Low-Cost Fecal Metabolome Sampling;** Alexey Melnik<sup>1,2</sup>; Alexander Aksekov<sup>1,2</sup>; <sup>1</sup>University of Connecticut, Storrs, CT; <sup>2</sup>Arome Science Inc., Farmington, CT
- TP 430 **Expanding metabolic coverage for sustained large-scale reversed-phase profiling of blood products using a novel dispersive solid phase extraction protocol;** Mark David<sup>1</sup>; Elena Chekmeneva<sup>1</sup>; Maria Gomez Romero<sup>1</sup>; Stephane Camuzeaux<sup>1</sup>; Benjamin Cooper<sup>1</sup>; Ada Armstrong<sup>1</sup>; Ravi Mehta<sup>1</sup>; Shiranee Srisakanda<sup>1</sup>; Miguel Reis Ferreira<sup>2</sup>; Olivier Cloarec<sup>3</sup>; Caroline Sands<sup>1</sup>; Goncalo Correia<sup>1</sup>; Zoltan Takats<sup>1</sup>; Matthew R Lewis<sup>1</sup>; <sup>1</sup>Imperial College London, London, United Kingdom; <sup>2</sup>King's College London, London, United Kingdom; <sup>3</sup>Sartorius Stedim Biotech GmbH, Goettingen, Germany
- TP 431 **Automated sample preparation using the Waters Andrew+ pipetting robot with biocrates' MxP@Quant 500 kit for high-throughput metabolomic profiling.;** Zachary J Mayer<sup>1</sup>; Stephen Dearth<sup>2</sup>; Timothy Griffin<sup>1</sup>; Giorgio Horak<sup>3</sup>; Vincent Bel<sup>3</sup>; Markus Langsdorf<sup>2</sup>; Candace Guerrero<sup>1</sup>; <sup>1</sup>Center for Metabolomics and Proteomics, University of Minnesota, Minneapolis, MN; <sup>2</sup>biocrates life sciences ag – Eduard-Bodem-Gasse 8, Innsbruck, Austria; <sup>3</sup>Waters Corporation, Eschborn, Germany
- TP 432 **Mass Spectrometry Detection of Root Exudate Metabolites by Filter Based Sampling;** Nilay Saha<sup>1</sup>; Alessandra Ceretto<sup>1</sup>; Cynthia Weing<sup>1</sup>; Franco Basile<sup>1</sup>; <sup>1</sup>University of Wyoming, Laramie, WY
- TP 433 **Easy-Omics: Taking the sweat out of metabolomics through automation;** Joshua P. Guerrette<sup>1</sup>; Erin Redman<sup>1</sup>;

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- Scott Mellors<sup>1</sup>; Sam Stewart<sup>1</sup>; J. Will Thompson<sup>1</sup>; <sup>1</sup>908 Devices Inc, Morrisville, NC
- TP 434 **Sample Preparation Optimization for Metabolomics Analysis of Cell Culture Media to Reduce Maillard Reaction Products**; Vyncent Nguyen<sup>1</sup>; Didar Asik<sup>1</sup>; Andy Campbell<sup>1</sup>; Jaime S Goldfuss<sup>1</sup>; Chengjian Tu<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Buffalo, NY
- TP 435 **---Extraction conditions impact recovery of specific metabolites in murine samples**; Amy Johnson<sup>1</sup>; Molly T. Soper-Hopper<sup>1</sup>; Rachel J. House<sup>1</sup>; Michael P. Vincent<sup>1</sup>; Abigail E. Ellis<sup>2</sup>; Christine N. Isaguirre<sup>2</sup>; Ryan D. Sheldon<sup>2</sup>; <sup>1</sup>Van Andel Research Institute, Grand Rapids; <sup>2</sup>Van Andel Research Institute, Grand Rapids, MI
- TP 436 **High-Throughput and Low-Input Metabolomics/Lipidomics Sample Preparation – A New BeatBox® Application**; Cameron Ellis<sup>1</sup>; Bryan Ngo<sup>2</sup>; Daniel Itzhak<sup>2</sup>; Junhua Wang<sup>2</sup>; Katharina Limm<sup>3</sup>; <sup>1</sup>PreOmics, Billerica, MA; <sup>2</sup>Altos Labs, Redwood City, California; <sup>3</sup>PreOmics GmbH, München, Germany
- TP 437 **Evaluation of Metabolomics of Dried Blood from Various Remote Sampling Technologies: Parameters of Acquisition, Extraction and Analysis**; Jiajun Lei<sup>1</sup>; Jonathan E. Katz<sup>1,2</sup>; <sup>1</sup>Ellison Institute of Technology, Los Angeles, CA; <sup>2</sup>University of Southern California, Los Angeles, CA
- METABOLOMICS: UNTARGETED METABOLITE PROFILING II**  
438-471
- TP 438 **Metabolomics-aided biomarker discovery and elucidation of molecular pathways**; Anthony Tsaropoulos<sup>1</sup>; Nikolaos Stavros Koulakiotis<sup>2</sup>; Evangelia Karkoula<sup>2</sup>; Ioanna Dagla<sup>2</sup>; Evagelos Gikas<sup>1</sup>; Nikolaos Kokras<sup>1</sup>; Christina Dalla<sup>1</sup>; <sup>1</sup>National and Kapodistrian University of Athens Medical School, Athens, Greece; <sup>2</sup>The Goulandris Natural History Museum, Kifissia, Greece, Kifissia, Greece
- TP 439 **Differential Metabolomics for Mouse Liver Induced by Microplastics Utilizing SWATH-based Mass Spectrometry**; Kuan-Lu Wu<sup>1</sup>; Sung-Fang Chen<sup>1</sup>; <sup>1</sup>National Taiwan Normal University, Taipei, Taiwan
- TP 440 **LC-MS/MS reveals kelp forest DOM composition and key insights into how algae exudates influence species interactions**; Shane Farrell<sup>1</sup>; Daniel Petras<sup>2</sup>; Dara Yiu<sup>1</sup>; Abzer K Pakkir Shah<sup>3</sup>; Aaron Hartmann<sup>4</sup>; John Burns<sup>1</sup>; Damian Brady<sup>5</sup>; Doug Rasher<sup>1</sup>; <sup>1</sup>Bigelow Laboratory for Ocean Sciences, East Boothbay, ME; <sup>2</sup>University of California Riverside, Department of Biochemistry, Riverside, CA; <sup>3</sup>University of Tuebingen, Center for Plant Molecular Biology, Tübingen, Germany; <sup>4</sup>Harvard University, Cambridge, MA; <sup>5</sup>University of Maine, Darling Marine Center, Walpole, ME
- TP 441 **Elucidating the protective mechanisms of oral hyaluronic acid against UV-induced skin damage: a metabolomic and lipidomic approach**; Matej Simek<sup>1</sup>; Vratislav Berka<sup>1</sup>; Lukáš Opálka<sup>2</sup>; Martina Bajerová<sup>3</sup>; Kateřina Lehká<sup>1</sup>; Iva Dolečková<sup>1</sup>; Lukáš Kubala<sup>3</sup>; <sup>1</sup>Contipro, Dolní Dobrouč, Czech Republic; <sup>2</sup>Faculty of Pharmacy, Hradec Králové, Czech Republic; <sup>3</sup>Institute of Biophysics, Brno, Czech Republic
- TP 442 **Untargeted LC-HRMS-based metabolomic profiling reveals distinct metabolomic profiles in patients with metabolic dysfunction-associated steatotic liver disease**; Qing Zhao<sup>1</sup>; Guoshou Teo<sup>1</sup>; Pradeep Narayanaswamy<sup>2</sup>; Will De Nardo<sup>3</sup>; Umur Keles<sup>4</sup>; Philipp Kaldis<sup>4</sup>; Matthew Watt<sup>3</sup>; Hyungwon Choi<sup>1</sup>; <sup>1</sup>National University of Singapore, Singapore, Singapore; <sup>2</sup>SCIEX, Singapore, Singapore; <sup>3</sup>The University of Melbourne, Melbourne, Australia; <sup>4</sup>Lund University, Lund, Sweden
- TP 443 **Feature Agnostic Metabolomics for Dose Range Finding Experiments in Sub-cytotoxic Doses of Common Pesticides in Primary Human Cells**; Madison Grace Thornhill<sup>1,2</sup>; Emilio S. Rivera<sup>1,2</sup>; Erick S. LeBrun<sup>1,2</sup>; Emilia A. Solomon<sup>2</sup>; Claire K. Sanders<sup>3</sup>; Tara Harvey<sup>1,2</sup>; Joshua D. Breidenbach<sup>1,2</sup>; Brett R. Blackwell<sup>1,2</sup>; Marc Alvarez<sup>2</sup>; Kes A. Luchini<sup>1,2</sup>; Abigale S Mikolitis<sup>1,2</sup>; Zachary J. Sasiene<sup>1,2</sup>; Ethan M. McBride<sup>1,2</sup>; Austin R. Anderson<sup>1,2</sup>; Lauren K. Heine<sup>1,2</sup>; Chi-Yen Tseng<sup>1,2</sup>; Jessica A. Salguero<sup>1,2</sup>; Francisca E. Rodriguez<sup>1,2</sup>; Salvatore J. Palmisano<sup>1,2</sup>; Jeremy Norris<sup>4</sup>; Phillip M. Mach<sup>1,2</sup>; Trevor G. Glaros<sup>1,2</sup>; <sup>1</sup>Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>3</sup>Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>4</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN
- TP 444 **Metabolomic Fingerprint of Leishmaniasis: Profiles of Cutaneous and Mucosal Leishmania species with and without endosymbiotic Leishmania RNA Virus (LRV)**; Joseane L P G Pavao<sup>1,2</sup>; Andrea Lafleur<sup>3</sup>; Mahbobeh Lesani<sup>2</sup>; Martin Olivier<sup>3</sup>; Laura-Isobel McCall<sup>1,2</sup>; <sup>1</sup>San Diego State University, San Diego, CA; <sup>2</sup>University of Oklahoma, Norman, OK; <sup>3</sup>The Research Institute of the McGill University Health Centre, Infectious Diseases and Immunity in Global Health Program, Montreal, Quebec
- TP 445 **Characterizing UVPD and HCD Fragmentation Patterns of Diverse Indolic Small Molecules to Aid in Surveying the “Indolome”**; Michael W Christopher<sup>1</sup>; Sunandini Yedla<sup>2</sup>; Bashar Amer<sup>2</sup>; Susan Bird<sup>2</sup>; Rahul Deshpande<sup>2</sup>; William Barshop<sup>2</sup>; Boone M. Prentice<sup>1</sup>; Brandon Bills<sup>2</sup>; Timothy J. Garrett<sup>1</sup>; <sup>1</sup>University of Florida Department of Chemistry, Gainesville, FL; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- TP 446 **A Novel Approach for Comprehensive Carboxylic Acid Profiling Utilizing Halogenated Derivatization and Liquid Chromatography-Trapped Ion Mobility Spectrometry-Mass Spectrometry**; Kaylie I. Kirkwood-Donelson<sup>1</sup>; Prashant Rai<sup>1</sup>; Michael B. Fessler<sup>1</sup>; Alan K. Jarmusch<sup>1</sup>; <sup>1</sup>National Institute of Environmental Health Sciences, Durham, NC
- TP 447 **Rapid Assessment of Metabolism by Electrochemistry/MS-Drugs, Xenobiotics, Plants**; Martin Eysberg<sup>1</sup>; Hendrik-Jan Brouwer<sup>2</sup>; Jean-Pierre Chervet<sup>2</sup>; <sup>1</sup>Antec Scientific, LLC, Boston, MA; <sup>2</sup>Antec Scientific, Alphen aan den Rijn, Netherlands
- TP 448 **Characterization of steroid conjugates by LC-MS/MS using collision-induced dissociation, electron activated dissociation and UV-photodissociation**; Lysi Ekmekci<sup>1</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>University of Geneva, Genève, Switzerland
- TP 449 **FERMENTATION SUBSTRATE OPTIMIZATION UTILIZING COMPARATIVE ANALYSES CAPABILITY OF DIFFERENT METABOLOMIC PLATFORMS**; Garima Agarwal<sup>1</sup>; Jeremy McFadden<sup>1</sup>; Chris Brown<sup>1</sup>; Michael Fethe<sup>1</sup>; <sup>1</sup>Corteva Agrisciences, Indianapolis, IN
- TP 450 **A Comprehensive Analysis of Monozygous and Dizygous Twin Pairs discordant for Type 1 Diabetes (T1D) through LC-MS/MS Metabolomics**; Elizabeth R Flammer<sup>1</sup>; Hali C. Broncucia<sup>2</sup>; Andrea K. Steck<sup>2</sup>; Stephen E. Gitelman<sup>3</sup>; Heba M. Ismail<sup>4</sup>; Timothy J. Garrett<sup>1</sup>; <sup>1</sup>University of Florida, Department of Chemistry, Gainesville, FL; <sup>2</sup>Barbara Davis Center for Diabetes, University of Colorado Anschutz Medical Campus, Aurora, CO; <sup>3</sup>Department of Pediatrics, Diabetes Center, University of California at San Francisco, San Francisco, CA; <sup>4</sup>Department of Pediatrics, Indiana University School of Medicine, Indianapolis, IN
- TP 451 **Molecular changes of stained teeth by hydrogen peroxide and peroxymonosulfate treatments**; Paulo Wender Portal Gomes<sup>1</sup>; Simone Zuffa<sup>1</sup>; Anelize Bauermeister<sup>1</sup>; Andrés Mauricio Caraballo-Rodríguez<sup>1</sup>; Haoqi Nina Zhao<sup>1</sup>; Helena Mannocho-Russo<sup>1</sup>; Cajetan Dogo-isonagie<sup>2</sup>; Om Patel<sup>2</sup>; Paloma Pimenta<sup>2</sup>; Jennifer Gronlund<sup>2</sup>; Stacey Lavender<sup>2</sup>; Shira Pilch<sup>2</sup>; Venda Maloney<sup>2</sup>; Michael North<sup>2</sup>; Pieter C. Dorrestein<sup>1</sup>; <sup>1</sup>University of

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- California San Diego, La Jolla, CA; <sup>2</sup>Colgate-Palmolive, Piscataway, NJ
- TP 452 **Selecting Optimal Internal Standards for Non-targeted LC-MS Metabolomics in a Large Core Facility;** Emilia J McCann<sup>1</sup>; Uri Keshet<sup>1</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>University of California Davis, Davis, CA
- TP 453 **A comprehensive Untargeted Fecal Metabolomics Workflow on the Orbitrap Astral MS to Achieve Deep Metabolome Coverage and Confident Compound Annotation;** Bashar Amer<sup>1</sup>; Yasin El Abiead<sup>2</sup>; Pieter C. Dorrestein<sup>2</sup>; Daniel Hermanson<sup>1</sup>; Susan Bird<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>University of California - San Diego, San Diego, California
- TP 454 **Demystifying microbore UHPLC-HRMS for sensitive and robust untargeted metabolomics;** Eduardo Sommella<sup>1</sup>; Danila La Gioia<sup>1, 2</sup>; Pietro Campiglia<sup>1</sup>; <sup>1</sup>University of Salerno, Fisciano (SA), Italy; <sup>2</sup>PhD Program in Drug Discovery and Development, University of Salerno, Fisciano, SA, Italy, Fisciano (SA), Italy
- TP 455 **Metabolomic Profiling of Osteocyte Extracellular Vesicles and Matrix Bound Vesicles using a Prototype Benchtop Multi Reflecting Time-of-Flight (MRT) Mass Spectrometer;** Lisa Reid<sup>1</sup>; Alicia Keenan<sup>2</sup>; Stephen Griffin<sup>3</sup>; Lee A Gethings<sup>1</sup>; Liam M Heaney<sup>2</sup>; Aveen Jalal<sup>2</sup>; Genevieve Anghileri<sup>2</sup>; Owen G Davies<sup>2</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>School of Sport, Exercise and Health Sciences, Loughborough University, Loughborough, United Kingdom; <sup>3</sup>Waters Corporation, Milford, Massachusetts
- TP 456 **Development of microfluid based UPLC-MS untargeted metabolomic methods for newborn screening;** Etienne Ljoni Poisson<sup>1</sup>; Freyr Jóhannsson<sup>2</sup>; Leifur Franzson<sup>3</sup>; Margrét Þorsteinsdóttir<sup>4</sup>; Jón Jóhannes Jónsson<sup>5</sup>; Ottar Rolfsson<sup>6</sup>; <sup>1</sup>University of Iceland, Reykjavik, Iceland; <sup>2</sup>Department of Genetics and Molecular Biology, Icelandic National Hospital, Reykjavik, Iceland; <sup>3</sup>Project Leader, Department of Clinical Biochemistry, Icelandic National Hospital, Reykjavik, Iceland; <sup>4</sup>Professor, Faculty of Pharmaceutical Sciences, University of Iceland, Director of R&D at ArcticMass, Reykjavik, Iceland; <sup>5</sup>Director of Genetics and Molecular Medicine, Icelandic National Hospital, Reykjavik, Iceland; <sup>6</sup>Professor at The Centre for Systems Biology, Medical School, University of Iceland, Reykjavik, Iceland
- TP 457 **Mass query language and collisional cross section prediction to support chemical derivatization research using mass spectrometry;** Jesba Bas Concepcion<sup>1</sup>; Jeffrey R Gilbert<sup>2</sup>; Chris Brown<sup>2</sup>; Sofie Weinkouff<sup>3</sup>; Dave Robbins<sup>2</sup>; Heiko Neuweger<sup>3</sup>; <sup>1</sup>Corteva, Whitestown, IN; <sup>2</sup>Corteva Agriscience, Indianapolis, IN; <sup>3</sup>Bruker Daltonics GmbH & Co. KG, Billerica, MA
- TP 458 **Untargeted metabolomics reveals secondary metabolites associated with fungal-fungal competition under select nutrient conditions;** Sameer Mudbhari<sup>1, 2</sup>; Jose Eduardo Marques Galvez<sup>3</sup>; Claire Veneault-Fourrey<sup>3</sup>; Robert L Hettich<sup>1, 2</sup>; Paul E Abraham<sup>1, 2</sup>; <sup>1</sup>The University of Tennessee Knoxville, Knoxville, TN; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>3</sup>INRAE-Université de Lorraine, Nancy, France
- TP 459 **Untargeted metabolomic profiling reveals process optimization strategies in a mock bioreactor;** Adam D Richardson<sup>1</sup>; Ethan Stancliffe<sup>1</sup>; Monil Gandhi<sup>1</sup>; Ashima Mehta<sup>1</sup>; Kevin Y Cho<sup>2</sup>; Gary J. Patti<sup>1, 2</sup>; <sup>1</sup>Panome Bio, St Louis, MO; <sup>2</sup>Washington University in St. Louis, St. Louis, MO
- TP 460 **Optimization of sample preparation and LC-MS analysis for high-throughput untargeted lipidomics and metabolomics;** Djawed Bennouna<sup>1</sup>; Christopher A LeClair<sup>1</sup>; Ewy Mathé<sup>1</sup>; <sup>1</sup>NIH/NCATS, Rockville, Maryland
- TP 461 **Expanding Normalization Coverage using Surrogate Metabolites in the Human Cell Metabolome;** Olivia Taverniti<sup>1</sup>; Brandon Y Lieng<sup>1</sup>; Jeremy K Chan<sup>1</sup>; William D Gwynne<sup>1</sup>; Andrew T Quail<sup>1</sup>; J. Rafael Montenegro-Burke<sup>1</sup>; <sup>1</sup>Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON
- TP 462 **Metabolomics and lipidomics approaches for the identification of HCC biomarkers in patients with liver cirrhosis;** Md Mamunur Rashid<sup>1</sup>; Rency S Varghese<sup>1</sup>; Habtom Resson<sup>1</sup>; <sup>1</sup>Georgetown University, Washington, DC
- TP 463 **Untargeted Metabolomics for Differential Analysis of Bacterial-Induced Sepsis;** Michael P Napoliitano<sup>1</sup>; Hong Wang<sup>1</sup>; Bruce A Kimball<sup>1</sup>; <sup>1</sup>Monell Chemical Senses Center, Philadelphia, PA
- TP 464 **Simultaneous Quantitation and Discovery (SQUAD) Liquid Chromatography Mass Spectrometry of Progesterone Steroids Relevant to Ovarian Cancer;** Elisabeth Schwiebert<sup>1</sup>; Samuel G. Moore<sup>1, 2</sup>; Jaeyeon Kim<sup>3</sup>; David A. Gaul<sup>1, 2</sup>; Facundo M. Fernández<sup>1, 2</sup>; <sup>1</sup>School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Petit Institute of Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA; <sup>3</sup>Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indiana University, Melvin and Bren Simon Comprehensive Cancer Center, Indianapolis, IN
- TP 465 **Juicy Insights: A Nontargeted, Standardized Metabolomics Approach for Comparing Apples to Apples;** Melanie Odenkirk<sup>1, 2</sup>; Margaret Read<sup>1</sup>; Cole Michel<sup>3</sup>; Katrina Doenges<sup>3</sup>; Jacqueline Michelle Chaparro<sup>1</sup>; Susan B Mitchell<sup>1</sup>; Nathan Montgomery<sup>1</sup>; Corey D Broeckling<sup>1</sup>; Sarah Brinkley<sup>4</sup>; Katrina L Leaprot<sup>5</sup>; Stacy D Sherrod<sup>5</sup>; Jody C May<sup>5</sup>; Juliana Chaura<sup>6</sup>; Gabriel E Velez Mejia<sup>6</sup>; Arpana Vaniya<sup>7</sup>; John A McLean<sup>5</sup>; Richard Reisdorph<sup>3</sup>; Nichole Reisdorph<sup>3</sup>; Andres Jaramillo-Botero<sup>6, 8</sup>; Oliver Fiehn<sup>7</sup>; Chi-Ming Chien<sup>2</sup>; Tracy Shafizadeh<sup>2</sup>; Jessica E Prenni<sup>1</sup>; Steve Watkins<sup>2</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO; <sup>2</sup>Verso Biosciences, Davis, CA; <sup>3</sup>University of Colorado, Anschutz Medical Campus, Department of Pharmaceutical Sciences, Aurora, CO; <sup>4</sup>The Alliance of Bioversity International & The International Center for Tropical Agriculture (CIAT), Cali, Colombia; <sup>5</sup>Vanderbilt University, Nashville, TN; <sup>6</sup>Pontificia Universidad Javeriana, Cali, Colombia; <sup>7</sup>University of California, Davis, Davis, California; <sup>8</sup>California Institute of Technology, Pasadena, CA
- TP 466 **High throughput plasma profiling of human liver disease samples using rapid chromatography and a multi-reflecting time-of-flight mass spectrometer;** Adam M King<sup>1</sup>; Ana S Lorenzo<sup>2</sup>; Yuriy Pyatkovskyy<sup>3</sup>; Emma Marsden-Edwards<sup>1</sup>; Elizabeth J Want<sup>2</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Imperial College London, London, United Kingdom; <sup>3</sup>Waters Corporation, Milford, Massachusetts
- TP 467 **Exploring Metabolites within Organoids and Organoids-on-Chips during Colorectal Cancer (CRC) Therapeutic Treatments;** Ethan Canfield<sup>1</sup>; Carly Strelez<sup>1</sup>; Rachel Perez<sup>1</sup>; Aaron Schatz<sup>1</sup>; Heinz-Josef Lenz<sup>2</sup>; Jonathan Katz<sup>1</sup>; Shannon Mumenthaler<sup>1</sup>; <sup>1</sup>Ellison Institute of Technology, Los Angeles, CA; <sup>2</sup>University of Southern California, Los Angeles, CA
- TP 468 **Advancing Metabolomics Analysis using GC-MS with Cold EI for Increased Identification, Throughput, and Sensitivity;** Luis M Valdiviez<sup>1</sup>; Uri Keshet<sup>1</sup>; Aviv Amirav<sup>2</sup>; Benjamin Neumark<sup>2</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>West Coast Metabolomics Center, University of California, Davis, Davis, CA; <sup>2</sup>Tel Aviv University, Tel Aviv, Israel
- TP 469 **A Multi-Omic Identification Protocol for High-Throughput Bacterial Analysis;** Jana M Carpenter<sup>1</sup>; Hannah Hynds<sup>1</sup>; Kingsley Bimpeh<sup>1</sup>; Kelly M. Hines<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- TP 470 **Utilizing liquid chromatography and mass spectrometry techniques for metabolic profiling of citrus parental varieties to inform breeding strategies;** Anil Bhatia<sup>1</sup>; Pallavi Agarwal<sup>2</sup>; Manhoi Hur<sup>1</sup>; Amancio J De Souza<sup>1</sup>; Chandrika Ramadugu<sup>2</sup>; <sup>1</sup>UCR Metabolomics Core, University of California, Riverside, California; <sup>2</sup>Department of

## TUESDAY POSTERS

- Botany and Plant Sciences, University of California, Riverside, CA
- TP 471 **Untargeted Exploration of Putative Emotional Chemo-Signals by thermal desorption preconcentration GC-EI&CI-TOFMS**; Marleen Vetter<sup>1</sup>; Eliska Ceznerova<sup>1</sup>; Sonja Klee<sup>1</sup>; Steffen Bräkling<sup>1</sup>; Megan Claffin<sup>2</sup>; Biagio D'Aniello<sup>3</sup>; Alfredo Di Lucrezia<sup>3</sup>; Anna Scandurra<sup>3</sup>; Claudia Pinelli<sup>4</sup>; Francesco Loreto<sup>5</sup>; Maurilia M. Monti<sup>6</sup>; Michelina Ruocco<sup>6</sup>; Gün R. Semin<sup>7</sup>; Luca Cappellin<sup>8</sup>; <sup>1</sup>TOFWERK, Thun, Switzerland; <sup>2</sup>Aerodyne Research Inc., Billerica, MA; <sup>3</sup>Univeristy of Naples Federico II, Napels, Italy; <sup>4</sup>University of Campania Luigi Vanvitelli, Caserta, Italy; <sup>5</sup>University of Naples Federico II, Napels, Italy; <sup>6</sup>Italian National Research Council (CNR), Naples, Italy; <sup>7</sup>William James center of research ISPA, Lisbon, Portugal; <sup>8</sup>University of Padua, Padua, Italy
- MICROORGANISMS AND THE MICROBIOME II**  
472-496
- TP 472 **MftP is a Multi-Drug Efflux Pump with a Vital Role in Regulating Cellular Homeostasis in Burkholderia thailandensis**; Ahmed Al-Tohamy<sup>1</sup>; Fabrizio Donnarumma<sup>1</sup>; Anne Grove<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA
- TP 473 **Spent media analysis and metabolic modeling-guided bioprocess optimization for recombinant protein production from E. colion complex media**; Hardik Dodia<sup>1</sup>; Vivek Mishra<sup>2</sup>; Charandatta Muddana<sup>2</sup>; Prajval Nakrani<sup>2</sup>; Pramod P. Wangikar<sup>1, 2</sup>; <sup>1</sup>Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai, India; <sup>2</sup>Clarity Bio Systems India Pvt. Ltd., Pune, India
- TP 474 **MetaLab: An Advanced Software Solution for Comprehensive DDA and DIA Metaproteomics Analysis on Multiple MS Platforms**; Kai Cheng<sup>1</sup>; Zhibin Ning<sup>1</sup>; Daniel Figeys<sup>1</sup>; <sup>1</sup>University of Ottawa, Ottawa
- TP 475 **Plasma metabolomics uncovers characteristic metabolic aberrancies in early-onset Crohn's Disease**; Zhiwei Zhou<sup>1</sup>; Yuanyuan Liu<sup>1</sup>; Ruben Colman<sup>1</sup>; Michael Rosen<sup>1</sup>; Michael Fischbach<sup>1</sup>; Dylan Dodd<sup>1</sup>; <sup>1</sup>Stanford University, Stanford, CA
- TP 476 **Plasmid-encoded colicin immunity proteins synthesized by pathogenic Escherichia coli identified by antibiotic induction, MALDI-TOF-TOF-MS/MS and top-down proteomic analysis**; Clifton K Fagerquist<sup>1</sup>; Yanlin Shi<sup>1</sup>; Jihyun Park<sup>1</sup>; <sup>1</sup>Produce Safety & Microbiology, Western Regional Research Center, Agricultural Research Service, USDA, Albany, CA
- TP 477 **The impact of MALDI-TOF-MS sampling rates on microbial identification results**; Ko Keng Chang<sup>1</sup>; Yi-Sheng Wang<sup>1</sup>; <sup>1</sup>Academia Sinica, Taipei, Taiwan
- TP 478 **A Simplified and Efficient Method for Expanding Gut Metaproteomic Coverage**; Pei-Chen Hsu<sup>1</sup>; Pei-Shan Wu<sup>2</sup>; Chuan-Chih Hsu<sup>3</sup>; Miao-Hsia Lin<sup>4</sup>; <sup>1</sup>Department of Microbiology, College of Medicine, National Taiwan University, Taipei City, Taiwan; <sup>2</sup>Department of Ophthalmology, National Taiwan University Hospital, College of Medicine, National Taiwan University, Taipei city, Taiwan; <sup>3</sup>Institute of Plant and Microbial Biology, Academia Sinica, Taipei city, Taiwan; <sup>4</sup>Department of Microbiology, College of Medicine, National Taiwan Univeristy, Taipei city, Taiwan
- TP 479 **Applying Untargeted Metabolomics to a Synthetic Cystic Fibrosis Microbial Community**; Emily C Giedraitis<sup>1</sup>; Rachel L Neve<sup>2</sup>; Vanessa V Phelan<sup>1</sup>; <sup>1</sup>Department of Pharmaceutical Sciences, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of Colorado-Anschutz Medical Campus, Aurora, CO; <sup>2</sup>Department of Immunology and Microbiology, School of Medicine, University of Colorado-Anschutz Medical Campus, Aurora, CO
- TP 480 **LC-MS/MS-based comparative analysis of N-glycome, proteome and glycoproteome of multiple Candida species point to the potential cause of high pathogenicity**; Sheryl Joyce B. Grijaldo-Alvarez<sup>1</sup>; Michael Russelle S. Alvarez<sup>1</sup>; Luiz Eduardo Lacerda<sup>2</sup>; Ricardo Wagner Portela<sup>2</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>University of California Davis, Davis, CA; <sup>2</sup>Universidade Federal da Bahia, Salvador, Brazil
- TP 481 **Protein O-glycosylation in the Bacteroidota phylum**; Dennis Svedberg<sup>1</sup>; Elisabeth Baland<sup>1</sup>; Lucía Perez<sup>1</sup>; Bolor Buyanbadrakh<sup>1</sup>; Shaochun Zhu<sup>1</sup>; Andre Mateus<sup>1</sup>; <sup>1</sup>Umeå University, Umeå, Sweden
- TP 482 **De Novo Library Construction for Metaproteomic Analyses of Human Datasets**; Andrew T Rajczewski<sup>1</sup>; Reid Wagner<sup>2</sup>; Subina P Mehta<sup>1</sup>; Tim Griffin<sup>1</sup>; Pratik Dilip Jagtap<sup>1</sup>; <sup>1</sup>University of Minnesota, Twin Cities, Minneapolis, MN; <sup>2</sup>Minnesota Supercomputing Institute, Minneapolis, MN
- TP 483 **Structural characterization of commensal bacteria-derived lipid As and elucidation of their impact on host immune responses**; Byoungsook Goh<sup>1</sup>; Ji-Sun Yoo<sup>1</sup>; Sungwhan F. Oh<sup>1, 2</sup>; <sup>1</sup>Brigham and Women's Hospital, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA
- TP 484 **Changes in Infant Health-Related Metabolites during Pregnancy After a Nutritional Intervention**; Emma R Guberson<sup>1</sup>; Elisa Caffrey<sup>1</sup>; Justin L Sonnenburg<sup>1, 2, 3</sup>; <sup>1</sup>Department of Microbiology and Immunology, Stanford University, Palo Alto, California; <sup>2</sup>Chan-Zuckerburg Biohub, San Francisco, California; <sup>3</sup>Center for Human Microbiome Studies, Stanford University, Palo Alto, CA
- TP 485 **Bacterioscore in 2D/3D MS imaging: pioneering in vivo cancer microbiome study and its link with diagnosis and patient survival**; Léa LEDOUX<sup>1</sup>; Yanis Zirem<sup>1</sup>; Michel Salzet<sup>1</sup>; Isabelle Fournier<sup>1</sup>; <sup>1</sup>PRISM - Inserm U1192, Villeneuve d'Ascq Cedex France, France
- TP 486 **Multi-omic network analysis identifies synergistic mechanisms for dietary lipids and microbiome pathobionts to drive macrophage innate immunity and metabolic disease**; Jacob W Pederson<sup>1,2</sup>; Jyothi Padiadpu<sup>2</sup>; Andrey Morgun<sup>2</sup>; Natalia Shulzhenko<sup>2</sup>; Aleksandra Nita-Lazar<sup>1</sup>; <sup>1</sup>NIAID, Bethesda, MD; <sup>2</sup>Oregon State University, Corvallis, OR
- TP 487 **Development of novel mouse models with improved translatability to the human microbiome**; Szymon Filip<sup>1</sup>; Greg Fedewa<sup>1</sup>; Cuong Nguyen<sup>1</sup>; Leslie Sedgeman<sup>1</sup>; Jasmine Chong<sup>1</sup>; Antonio Carmona<sup>1</sup>; Miriam Velez<sup>1</sup>; Nathan Wan<sup>1</sup>; Yan Yang<sup>1</sup>; Sarkis Mazmanian<sup>2</sup>; Bryan Yoo<sup>1</sup>; <sup>1</sup>Nuanced Health, Los Angeles, CA; <sup>2</sup>California Institute of Technology, Pasadena, CA
- TP 488 **A multimodal platform for lipid A structural analysis from a single colony**; Hyojik Yang<sup>1</sup>; Ian O'Keefe<sup>1</sup>; Richard D. Smith<sup>1</sup>; Kylie P. Sumner<sup>1</sup>; Matthew E. Sherman<sup>1</sup>; DAVID R GOODLETT<sup>2</sup>; Charles R. Sweet<sup>3</sup>; ROBERT K ERNST<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore, MD; <sup>2</sup>University of Victoria, Victoria, BC; <sup>3</sup>United States Naval Academy, Annapolis, MD
- TP 489 **Beyond the Biotype: leveraging LC-MS proteomics to systematically map the proteomes of 38,000 bloodstream infection isolates**; Annegret Ulke-Lemee<sup>1</sup>; Rory Gilliland<sup>1</sup>; Mario Valdés-Tresanco<sup>1</sup>; Morgan Hepburn<sup>1</sup>; Ryan Groves<sup>1</sup>; Anika Westlund<sup>1</sup>; Andriy Plakhotnyk<sup>1</sup>; Gopal Ramamourthy<sup>1</sup>; Daniel Gregson<sup>2</sup>; Thi Mui Pham<sup>3</sup>; Tatum Mortimer<sup>4</sup>; Joshua Smith<sup>5</sup>; Bruce Walker<sup>6</sup>; Yonatan Grad<sup>3</sup>; Ashlee Earl<sup>5</sup>; Hallgrímur Benediktsson<sup>1</sup>; Ethan MacDonald<sup>1</sup>; Ian Lewis<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, AB; <sup>2</sup>Alberta Provincial Laboratories, Calgary, AB; <sup>3</sup>Harvard T.H. Chan School of Public Health, Boston, MA; <sup>4</sup>University of Georgia, Athens, GA; <sup>5</sup>Broad Institute, Cambridge, MA
- TP 490 **Stabilizing the Mycobacterial Small Proteome Through Proteasome Inhibition**; Hannah A. Marietta<sup>1</sup>; Simon D Weaver<sup>1</sup>; Taylor J. Lundgren<sup>1</sup>; Patricia L. Clark<sup>1</sup>; Matthew M. Champion<sup>1</sup>; <sup>1</sup>University of Notre Dame, Notre Dame, IN
- TP 491 **LC-MS as a platform for precision medicine: predicting survival from bloodstream infections using a training set of 38,000 microbial proteomes**; Rory Gilliland<sup>1</sup>; Ashlee Earl<sup>2</sup>; Anika Westlund<sup>1</sup>; Bruce Walker<sup>2</sup>; Andriy Plakhotnyk<sup>1</sup>; Annegret Ulke-Lemee<sup>1</sup>; Colin Mackenzie<sup>1</sup>; Morgan

## TUESDAY POSTERS

- Hepburn<sup>1</sup>; Thi Mui Pham<sup>3</sup>; Gopal Ramamourthy<sup>1</sup>; Yonatan Grad<sup>3</sup>; Hallgrimur Benediktsson<sup>1</sup>; Ethan MacDonald<sup>1</sup>; [Ian Lewis](#)<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, AB; <sup>2</sup>Broad Institute, Cambridge, MA; <sup>3</sup>Harvard T.H. Chan School of Public Health, Boston, MA
- TP 492 **Application of a microbiome-specific metabolite library in untargeted plasma metabolomics**; [Jaclyn Weinberg](#)<sup>1</sup>; William Crandall<sup>1</sup>; Anthony Gacasan<sup>1</sup>; Sami Teeny<sup>1</sup>; James Zhan<sup>1</sup>; Rheinallt Jones<sup>1</sup>; Michael Woodworth<sup>1</sup>; Dean Jones<sup>1</sup>; <sup>1</sup>Emory University, Atlanta, GA
- TP 493 **The virus microenvironment in 2D and 3D: Intercellular communication guides tumor-specific vulnerabilities to viral infection**; Krystal K. Lum<sup>1</sup>; James C. Kostas<sup>1</sup>; Colter Brainard<sup>1</sup>; Oscar Pundel<sup>2</sup>; Qingwen Jiang<sup>3</sup>; Karuna Ganesh<sup>3</sup>; Benjamin G. Neel<sup>2</sup>; [Ileana M. Cristea](#)<sup>1</sup>; <sup>1</sup>Princeton University, Princeton, NJ; <sup>2</sup>NYU Langone, New York, NY; <sup>3</sup>Memorial Sloan Kettering Cancer Center, New York, NY
- TP 494 **From Dirt to Data: Comparing Liquid Chromatography-Mass Spectrometry Methods for Low-Biomass Soil Metaproteomics**; [Doratheia Lee](#)<sup>1</sup>; Gustavo Diaz<sup>1</sup>; Valerie A Seitz<sup>2</sup>; Mikayla A Borton<sup>3</sup>; Meagan E Schipanski<sup>3</sup>; Jessica E Prenni<sup>2</sup>; Kelly C Wrighton<sup>3</sup>; Corey D Broeckling<sup>1</sup>; <sup>1</sup>Analytical Resources Core: Bioanalysis and Omics Center, Colorado State University, Fort Collins, CO; <sup>2</sup>Department of Horticulture and Landscape Architecture, Fort Collins, CO; <sup>3</sup>Department of Soil and Crop Sciences, Colorado State University, Fort Collins, CO
- TP 495 **Aspergillus fumigatus secretes gliotoxin in response to polymycovirus infection**; Rutuja H Patil<sup>1</sup>; Amer Ali Abd El-Hafeez<sup>2</sup>; Gabriele Sass<sup>3</sup>; David A. Stevens<sup>2</sup>; Andrea Palyzová<sup>4</sup>; Joe Hsu<sup>2</sup>; Ioly Kotta-Loizou<sup>5</sup>; [Vladimír Havlíček](#)<sup>1</sup>; <sup>1</sup>Institute of Microbiology of the Czech Academy of Sciences, 142 20, Prague, Czech Republic; <sup>2</sup>Stanford University, Stanford, CA; <sup>3</sup>California Institute for Medical Research, San Jose, CA; <sup>4</sup>Institute of Microbiology of the Czech Academy of Sciences, Prague, Czech Republic; <sup>5</sup>Imperial College London, London, United Kingdom
- TP 496 **A Targeted Multi-Omics Platform for Characterizing Prebiotic-Probiotic Interactions**; [Christopher Suarez](#)<sup>1</sup>; Cheng-Yu Charlie Weng<sup>1</sup>; Karen Kalanetra<sup>2</sup>; Sarah Blecksmith<sup>3</sup>; Danielle Lemay<sup>3</sup>; David A. Mills<sup>2</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of California, Davis, Davis, California; <sup>2</sup>Department of Food Science and Technology, University of California Davis, Davis, CA; <sup>3</sup>Department of Nutritional Biology, University of California, Davis, Davis, CA
- NANOSCALE/MICROFLUIDIC AND CAPILLARY ELECTROPHORESIS SEPARATIONS AND MS**  
497-509
- TP 497 **Rapid Comparative Analysis of Glatiramer Acetate Products with CZE-MS**; [Joshua Shipman](#)<sup>1</sup>; A M Abdullah<sup>1</sup>; Cynthia Sommers<sup>1</sup>; Jason Rodriguez<sup>1</sup>; <sup>1</sup>Office of Pharmaceutical Quality Research, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Saint Louis, MO
- TP 498 **Comparing the merits of capillary electrophoresis versus microfluidic capillary electrophoresis in the bottom-up characterization of larger nucleic acids**; [Daniele Rollo](#)<sup>1</sup>; Daniele Fabris<sup>1</sup>; <sup>1</sup>University of Connecticut, Storrs, CT
- TP 499 **Coupling icIEF to high-resolution mass spectrometry for in-depth characterization of complex protein charge heterogeneity**; Teresa Kwok<sup>1</sup>; Tia Chan<sup>1</sup>; [Matthew Courtney](#)<sup>1</sup>; Tong Chen<sup>1</sup>; Tao Bo<sup>1</sup>; <sup>1</sup>Advanced Electrophoresis Solutions, Cambridge, ON
- TP 500 **Capillary Electrophoresis Miniature Mass Spectrometry System for Rapid and Sensitive Clinical Analysis**; Min Dang<sup>1</sup>; [Jiexun Bu](#)<sup>2</sup>; Junhan Wu<sup>1</sup>; Xiao Chen<sup>3</sup>; Wenpeng Zhang<sup>3</sup>; Zheng Ouyang<sup>3</sup>; <sup>1</sup>PURSPEC Technology (China) Ltd., Suzhou, China; <sup>2</sup>PURSPEC Technology (Beijing) Ltd., Beijing, China; <sup>3</sup>Tsinghua University, Beijing, China
- TP 501 **Characterization of Adeno-Associated Virus Capsids by a Novel Capillary Isoelectric Focusing-Based Fractionation Method and Charge Detection Mass Spectrometry**; Jiaqi Wu<sup>1</sup>; Benjamin Draper<sup>2</sup>; [Chris Heger](#)<sup>1</sup>; <sup>1</sup>Bio-Techne, San Jose, CA; <sup>2</sup>Megadallon Solutions, Bloomington, Indiana
- TP 502 **Coupling a 3D-Printed Herringbone Device to cVSSI-MS for Reaction Kinetic Studies**; [Amanda DeVor](#)<sup>1</sup>; Jing Wang<sup>1</sup>; Olanrewaju Awoyemi<sup>1</sup>; Sydney Anderson<sup>1</sup>; Peng Li<sup>1</sup>; Stephen J Valentine<sup>1</sup>; <sup>1</sup>West Virginia University- C. Eugene Bennett Department of Chemistry, Morgantown, WV
- TP 503 **Mass spectrometry-based top-down proteomics in nanomedicine: proteoform-specific measurement of nanoparticle protein corona**; Amirhossein Sadeghi<sup>1</sup>; Ali Akbar Ashkarran<sup>1</sup>; Morteza Mahmoudi<sup>1</sup>; Liangliang Sun<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI
- TP 504 **A Workflow for Antibody Charge Variant Fractionation Enabling CZE-MS**; [Jiaqi Wu](#)<sup>1</sup>; Scott J Mellors<sup>2</sup>; Will McElroy<sup>1</sup>; Chris Heger<sup>1</sup>; <sup>1</sup>Bio-Techne, San Jose, CA; <sup>2</sup>908 Devices Inc., Boston, MA
- TP 505 **Fractionation of Bispecific Antibody Charge Variants by MauriceFlex™ and their Identification by Mass Spectrometry**; [Srinivasa Rao](#)<sup>1</sup>; Andreas Nagel<sup>2</sup>; Chris Heger<sup>1</sup>; <sup>1</sup>Bio-Techne, San Jose, CA; <sup>2</sup>Genovis AB, Kävlinge, Sweden
- TP 506 **Optimization of Capillary Electrophoresis Mass spectrometry for Carbene Chemical Footprinting Analysis**; [Daoyang Chen](#)<sup>1</sup>; Laurence Fayadat-Dilman<sup>1</sup>; Jason Hogan<sup>1</sup>; <sup>1</sup>Merck, South San Francisco, CA
- TP 507 **Development of highly sensitive sheathless CE-MS method and application to small volume cell analysis**; [Akiyoshi Hirayama](#)<sup>1, 2</sup>; Kenichi Takahashi<sup>1</sup>; Tomoyoshi Soga<sup>1</sup>; <sup>1</sup>Keio University, Tsuruoka, Japan; <sup>2</sup>INCEMS Technologies, Co. Ltd., Tsuruoka, Japan
- TP 508 **Single-Cell Metabolomic Characterization via CE-NanoESI-MS with Nanoflow Sheath Liquid Interface**; [Shuangshuang Chen](#)<sup>1</sup>; Mike Knierman<sup>2</sup>; Stanislav Rubakhin<sup>1</sup>; Noah A. Bender<sup>1</sup>; Yash Nelavelli<sup>1</sup>; Jonathan V Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois Urbana Champaign, Urbana, IL; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- TP 509 **On-demand Mass Spectrometry for Modern Biopharmaceutical Workflows**; Austin Culbertson<sup>1</sup>; Mason A Chilmonczyk<sup>1</sup>; <sup>1</sup>Andson Biotech Inc., Atlanta, GA
- NEUROSCIENCE AND NEURODEGENERATIVE DISEASE RESEARCH I**  
510-530
- TP 510 **Quantification of brain cholesterol and cholesterol metabolites regulation during demyelination and remyelination in a genetic mouse model**; [Hudihim MWDK Dedunupitiya](#)<sup>1</sup>; Eden Parreno Go<sup>1</sup>; Nishama De Silva Mohotti<sup>1</sup>; Jenna Marie Williams<sup>1</sup>; Hiroko Kobayashi<sup>1</sup>; Rashmi Basavaraj Binjawadagi<sup>1</sup>; Heather Desaire<sup>1</sup>; Meredith Hartley<sup>1</sup>; <sup>1</sup>University of Kansas, Lawrence, KS
- TP 511 **Probabilistic graphical modeling approaches identify disease-specific features within complex lipidomic data from Parkinson's disease patient specimens**; [Nathan G. Hatcher](#)<sup>1</sup>; Dimitris V. Manatakis<sup>1</sup>; Nanyan R. Zhang<sup>1</sup>; Lihang Yao<sup>1</sup>; Cheryl E. G. Leyns<sup>1</sup>; Matthew J. Fell<sup>1</sup>; Kim Ekroos<sup>2</sup>; Jacob N. Marcus<sup>1</sup>; Smith M. Smith<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., Rahway, NJ; <sup>2</sup>Lipidomics Consulting Ltd., Esbo, Finland
- TP 512 **Integrated Proteomic and Transcriptomic Profiling Reveals Diversity of Hippocampal Subregions and Strata at Synaptic Resolution**; [Quinn Waselenchuk](#)<sup>1, 2, 3</sup>; Eva Kaulich<sup>1</sup>; Nicole Fürst<sup>1</sup>; Kristina Desch<sup>1, 2</sup>; Julian D. Langer<sup>1, 2</sup>; Erin M. Schuman<sup>1</sup>; <sup>1</sup>Max Planck Institute for Brain Research, Frankfurt, Germany; <sup>2</sup>Max Planck Institute of Biophysics, Frankfurt, Germany; <sup>3</sup>International Max Planck Research School on Cellular Biophysics, Frankfurt, Germany
- TP 513 **Spatial proteomic characterization of single amyloid plaque in murine Alzheimer's disease brains by laser capture microdissection and mass spectrometry**

## TUESDAY POSTERS

- Mengqi Chu<sup>1</sup>; Ju Wang<sup>1</sup>; Yun Jiao<sup>1</sup>; Junmin Peng<sup>1</sup>; <sup>1</sup>*St Jude children research hospital, Memphis, TN*
- TP 514 **Cholesterol ester dynamics during demyelination and remyelination**; Nishama Da Silva Mohotti<sup>1</sup>; Hiroko Kobayashi<sup>1</sup>; Jenna M. Williams<sup>1</sup>; Meredith D Hartley<sup>1</sup>; <sup>1</sup>*University of Kansas, Lawrence, KS*
- TP 515 **Mass spectrometry approach to characterize tumor heterogeneity in glioblastoma blood-brain-barrier 3D microtissues**; Maxine Lam<sup>1</sup>; Joey Aw<sup>1</sup>; Damien Tan<sup>2</sup>; Tianyun Zhao<sup>1</sup>; Andrea Pavesi<sup>1</sup>; Radoslaw Sobota<sup>2</sup>; <sup>1</sup>*A\*STAR, Singapore, Singapore*; <sup>2</sup>*A\*STAR, Singapore, Singapore*
- TP 516 **Neurogenesis-related proteomics modulation in germline histone H3.3 mutations**; Elizabeth G. Porter<sup>1</sup>; Francisca N De Luna Vitorino<sup>1</sup>; Khadija D. Wilson<sup>2</sup>; Yixuan Xie<sup>1</sup>; Peter Klein<sup>2</sup>; Elizabeth J. Bhoj<sup>2</sup>; Benjamin A Garcia<sup>1</sup>; <sup>1</sup>*Washington University School of Medicine, St. Louis, MO*; <sup>2</sup>*University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*
- TP 517 **Characterization of proteome and histone post-translational modification (PTM) changes associated with N-terminal neuroepigenetic histone mutations**; Carolina Brás Costa<sup>1</sup>; Francisca N. L. Vitorino<sup>1</sup>; Joanna K Lempiainen<sup>1</sup>; Elizabeth G. Porter<sup>1</sup>; Benjamin A Garcia<sup>1</sup>; <sup>1</sup>*Washington University School of Medicine, St. Louis, MO*
- TP 518 **Proteomic Analysis of Synaptosomes in a Huntington's Disease Mouse Model Reveals Pathological Contributions of Calcium/Calmodulin-Dependent Protein Kinase Type II**; Joanna Bons<sup>1</sup>; Maria A. Sanchez<sup>1</sup>; Elena T. Battistoni<sup>1</sup>; Barbara J. Bailus<sup>1</sup>; Swati Naphade<sup>1</sup>; Ningzhe Zhang<sup>1</sup>; Carlos Galicia Aguirre<sup>1</sup>; Lei Wei<sup>1</sup>; Ryan Quinn<sup>1</sup>; Lisa M. Ellerby<sup>1</sup>; Birgit Schilling<sup>1</sup>; <sup>1</sup>*Buck Institute for Research on Aging, Novato, CA*
- TP 519 **Phosphoproteomic characterization of the dorsal anterior cingulate cortex in Schizophrenia implicates CDK1 as a regulatory enzyme in psychiatric disease**; Andrew G. DeMarco<sup>1</sup>; Ryan Salisbury<sup>1</sup>; Kevin Xu<sup>1</sup>; Jordan Gilardi<sup>1</sup>; Akayla Lewin<sup>1</sup>; Lambertus Klei<sup>1</sup>; Robert A Sweet<sup>1</sup>; David A Lewis<sup>1</sup>; Bernie Devlin<sup>1</sup>; Matthew L MacDonald<sup>1, 2</sup>; <sup>1</sup>*Department of Psychiatry, University of Pittsburgh, Pittsburgh, PA*; <sup>2</sup>*Health Sciences Mass Spectrometry Core, University of Pittsburgh, Pittsburgh, PA*
- TP 520 **Electrophysiology-Assisted Single-Neuron Proteomics Reveals Gender Differences in Proteome Profile in the Locus Coeruleus of the Adult Mouse**; Jingyun Lee<sup>1</sup>; Zhong-Min Wang<sup>1</sup>; Maria Laura Messi<sup>1</sup>; Carol Milligan<sup>1</sup>; Cristina Maria Furdul<sup>1</sup>; Osvaldo Delbono<sup>1</sup>; <sup>1</sup>*Wake Forest University School of Medicine, Winston-Salem, NC*
- TP 521 **An optimized protocol for the preparation of protein-dextran mixtures for mass spectrometry-based proteomics analysis of microperfusates**; Xiaoli Wang<sup>1</sup>; M Cristine C. Charlesworth<sup>1</sup>; Cecile Riviere-Cazaux<sup>1</sup>; Benjamin J. Madden<sup>1</sup>; Kenneth L. Johnson<sup>1</sup>; Terry C. Burns<sup>1</sup>; Akhilesh Pandey<sup>1</sup>; Jun Zhong<sup>1</sup>; <sup>1</sup>*Mayo Clinic, Rochester, MN*
- TP 522 **Age-dependent changes in the molecular signatures of mouse brain elucidated by multi-protease proteomic and phosphoproteomic analyses**; Rodrigo Mohallem<sup>1</sup>; Allison J. Schaser<sup>1</sup>; Uma K. Aryal<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*
- TP 523 **Unveiling the Proteome Signatures of Traumatic Brain Injury Development and Progression in Small Extracellular Vesicles**; Mojibola O Fowowe<sup>1</sup>; Cristian D Gutierrez-Reyes<sup>1</sup>; Moyinoluwa Adeniyi<sup>1</sup>; Sherifdeen B Onigbinde<sup>1</sup>; Ayobami Oluokun<sup>1</sup>; Firas Kobeissy<sup>2</sup>; Stefania Mondello<sup>3</sup>; Ava M Puccio<sup>4</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>*Texas Tech University, Lubbock, TX*; <sup>2</sup>*Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA*; <sup>3</sup>*Department of Biomedical and Dental Sciences and Morphofunctional Imaging, University of Messina, Messina, Italy*; <sup>4</sup>*Department of Neurological Surgery, University of Pittsburgh, Pittsburgh, PA*
- TP 524 **Optimization of isolating synaptic vesicles for comprehensive glycoproteomic and neuropeptidomic analysis in neurodevelopmental disorders**; Julia L Hoffman<sup>1</sup>; Thao U Duong<sup>1</sup>; Elliot Patrenets<sup>2</sup>; Hannah N Miles<sup>3</sup>; Ashley Phetsanthad<sup>1</sup>; Pamela R Westmark<sup>4, 5</sup>; Cara J Westmark<sup>4, 5</sup>; Lingjun Li<sup>1, 3, 5</sup>; <sup>1</sup>*University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin*; <sup>2</sup>*University of Wisconsin-Madison, Department of Integrative Biology, Madison, Wisconsin*; <sup>3</sup>*University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin*; <sup>4</sup>*University of Wisconsin-Madison, Department of Neurology, Madison, Wisconsin*; <sup>5</sup>*University of Wisconsin-Madison, Molecular Environmental Toxicology Center, Madison, Wisconsin*
- TP 525 **Detection and characterization of Alzheimer's Disease biomarkers using Liquid Chromatography Ion Mobility Mass spectrometry (LC-IM-MS/MS)**; Kimberly Y. Kartowikromo<sup>1</sup>; Zachary E. Love<sup>1</sup>; Orobola E. Olajide<sup>1</sup>; Ahmed M. Hamid<sup>1</sup>; <sup>1</sup>*Auburn University, AUBURN, AL*
- TP 526 **Analysis of Anterior Cerebral Artery and Cortex Tissue in Alzheimer's Disease**; Margaret Downs<sup>1</sup>; Ashley Tai<sup>1</sup>; Thor D. Stein<sup>2, 3, 4</sup>; Yanhang Zhang<sup>5, 6, 7</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup>*Boston University Chobanian & Avedisian School of Medicine, Boston, MA*; <sup>2</sup>*Pathology and Laboratory Medicine, Boston University, Boston, MA*; <sup>3</sup>*VA Boston Healthcare system, U.S. Department of Veteran Affairs, Jamaica Plain, MA*; <sup>4</sup>*VA Bedford Healthcare System, US Department of Veteran Affairs, Bedford, MA*; <sup>5</sup>*Department of Mechanical Engineering, Boston University, Boston, MA*; <sup>6</sup>*Department of Biomedical Engineering, Boston University, Boston, MA*; <sup>7</sup>*Division of Materials Science and Engineering, Boston University, Boston, MA*
- TP 527 **Elucidating cellular and molecular features of white matter hyperintensities in Alzheimer's disease with multimodal imaging**; Claire F Scott<sup>1</sup>; Cody R Marshall<sup>2, 3</sup>; Madeline E Colley<sup>3, 4</sup>; Elena Solopova<sup>5</sup>; Lukasz Migas<sup>6</sup>; Angela R.S. Kruse<sup>3, 7</sup>; Katerina V Djambazova<sup>3, 7</sup>; Wilber Romero Fernandez<sup>5</sup>; Matthew S Schrag<sup>5</sup>; Raf Van De Plas<sup>6</sup>; Jeffrey M Spraggins<sup>2, 3, 4, 7, 8</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN*; <sup>3</sup>*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*; <sup>4</sup>*Department of Biochemistry, Vanderbilt University, Nashville, TN*; <sup>5</sup>*Department of Neurology, Vanderbilt University, Nashville, TN*; <sup>6</sup>*Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands*; <sup>7</sup>*Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN*; <sup>8</sup>*Department of Chemistry, Vanderbilt University, Nashville, TN*
- TP 528 **Overexpression of hSOD1G37R ALS mutant within the spinal cord of mice is characterized by proteomic changes linked to microglial activation**; Lester S. Manly<sup>1</sup>; Anne M. Roberts<sup>1</sup>; Eric B. Dammer<sup>2</sup>; Ankit P. Jain<sup>1</sup>; Nicholas T. Seyfried<sup>1, 2</sup>; Peter J. Crouch<sup>3</sup>; Blaine R. Roberts<sup>1, 2</sup>; <sup>1</sup>*Department of Biochemistry, Emory University, Atlanta, GA*; <sup>2</sup>*Department of Neurology, Emory University, Atlanta, GA*; <sup>3</sup>*School of Biomedical Sciences, University of Melbourne, Melbourne, Australia*
- TP 529 **Novel brain-penetrant inhibitor of G9a methylase blocks Alzheimer's disease proteopathology for precision medication**; Ling Xie<sup>1</sup>; Ryan Nicholas Sheehy<sup>1</sup>; Yan Xiong<sup>2</sup>; Adil Muneer<sup>3</sup>; Jin Jian<sup>2</sup>; Juan Song<sup>1</sup>; Xian Chen<sup>1</sup>; <sup>1</sup>*University of North Carolina at Chapel Hill, Chapel Hill, NC*; <sup>2</sup>*Icahn School of Medicine at Mount Sinai, New York, NY*; <sup>3</sup>*University of North Carolina Chapel Hill, Chapel Hill, NC*
- TP 530 **Psychedelics-induced proteomic alterations within the brain**; Kacper Lukasiewicz<sup>1</sup>; Tomasz Kowalczyk<sup>1</sup>; Arkadiusz Zbikowski<sup>1</sup>; Napoleon Waszkiewicz<sup>1</sup>; Adam Kretowski<sup>1</sup>; Michal Ciborowski<sup>1</sup>; Dominik Cysewski<sup>1</sup>; <sup>1</sup>*Medical University of Białystok, BIALYSTOK, Poland*



## TUESDAY POSTERS

- TP 531 **Streamlined IP-RP-LCMS workflow for siRNA characterization and routine impurity profiling;** CHEN-CHUN CHEN<sup>1</sup>; Matt Sorensen<sup>2</sup>; Todd Maloney<sup>2</sup>; <sup>1</sup>*Eli Lilly and Company, Indianapolis, IN*; <sup>2</sup>*Eli Lilly & Company, Indianapolis, IN*
- TP 532 **Negative Electron Transfer Collision-Induced Dissociation of G-quadruplexes: Uncovering the Guanine Radical Anion Loss Pathway;** Nicole M Brundridge<sup>1</sup>; Jordan M Fritz<sup>1</sup>; Jonathan Dickerhoff<sup>1</sup>; Danzhou Yang<sup>1</sup>; Scott A McLuckey<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*
- TP 533 **Rapid Oligonucleotide Separation and Sequence Confirmation Using Untargeted LC-UV-MS/MS and a New Data Analysis Software;** Katherine Sanders<sup>1</sup>; Amber Henry<sup>1</sup>; Kevin Ray<sup>1</sup>; <sup>1</sup>*Millipore Sigma, St. Louis, MO*
- TP 534 **Evaluation of Novel Triplex-Binding Ligands Using Native Mass Spectrometry;** Landy Gu<sup>1</sup>; Nghia Tran<sup>1</sup>; Vanessa Marie Rangel<sup>1</sup>; Liang Xue<sup>1</sup>; <sup>1</sup>*University of The Pacific, Stockton, CA*
- TP 535 **Investigation on Naturally Occurring Flavonoids on Their Ability to Stabilize DNA Triplexes;** Nghia T Tran<sup>1</sup>; Landy Gu<sup>1</sup>; Vanessa Rangel<sup>2</sup>; Tiffanie Jiang<sup>2</sup>; Holly Jiang<sup>2</sup>; Sabrina Ton<sup>2</sup>; Justin Shen<sup>2</sup>; Polina Eidelberg<sup>2</sup>; Liang Xue<sup>2</sup>; <sup>1</sup>*University of The Pacific, Stockton, CA*; <sup>2</sup>*University of the Pacific, Stockton, CA*
- TP 536 **Proximity proteomics profiling of RNA G-quadruplex-interacting proteins in live cells;** Xiaochen Liang<sup>1</sup>; Feng Tang<sup>2</sup>; Yinsheng Wang<sup>2</sup>; <sup>1</sup>*University of California Riverside, Riverside, CA*; <sup>2</sup>*University of California, Riverside, Riverside, CA*
- TP 537 **HPLC Fractionation and LCMS/MS Characterization of Human tRNA species;** Jennifer Kist<sup>1</sup>; Patrick A. Limbach<sup>1</sup>; <sup>1</sup>*University of Cincinnati, Cincinnati, OH*
- TP 538 **Analysis of RNA epigenetic modifications in peripheral white blood cells by mass spectrometry;** Cheng Guo; *Zhejiang University, Hangzhou, China*
- TP 539 **A mass spectrometry-based pipeline for identifying RNA modifications involved in cancer cell adaptation;** Aurore ATTINA<sup>1</sup>; Amandine Amalric<sup>2</sup>; Jérôme Vialaret<sup>1</sup>; Sylvain Lehmann<sup>1</sup>; Alexandre David<sup>3</sup>; Christophe Hirtz<sup>1</sup>; <sup>1</sup>*LBPC-PPC, Montpellier University, IRMB CHU Montpellier, INM INSERM, Montpellier, France*; <sup>2</sup>*IGF, INSERM, CNRS, MONTPELLIER, France*; <sup>3</sup>*Montpellier Cancer Research Institute, INSERM Montpellier, MONTPELLIER, France*
- TP 540 **Evaluation of crosslinked peptide-RNA oligonucleotides by NanoLC-ESI-MS/MS to Identify the Sequence and Position of the Crosslinked RNA;** Sinem Apaydin<sup>1</sup>; Aleksandar Chernev<sup>1</sup>; Ralf Pflanz<sup>1</sup>; Monika Raabe<sup>1</sup>; Henning Urlaub<sup>1, 2</sup>; <sup>1</sup>*Bioanalytical Mass Spectrometry Group, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany*; <sup>2</sup>*Bioanalytics Group, Department for Clinical Chemistry, University Medical Center Göttingen, Goettingen, Germany*
- TP 541 **Characterisation of small RNA-based therapeutics by fast, sensitive, and reproducible low flow LC-MS/MS method;** Silvia Millan Martin<sup>1</sup>; Felipe Guapo<sup>1</sup>; Nora Crushell<sup>1</sup>; Sara Carillo<sup>1</sup>; Ken Cook<sup>2</sup>; Alexander Boris Schwahn<sup>3</sup>; Shanhua Lin<sup>4</sup>; Jonathan Bones<sup>1, 5</sup>; <sup>1</sup>*The National Institute for Bioprocessing Research & Training, Dublin, Ireland*; <sup>2</sup>*Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*; <sup>3</sup>*Thermo Fisher Scientific, Reinach, Switzerland*; <sup>4</sup>*Thermo Fisher Scientific, Sunnyvale, CA*; <sup>5</sup>*School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland*
- TP 542 **Method considerations for therapeutic ASO RNA analysis. Adducts and insource impurity generation;** Ken Cook<sup>1</sup>; Ulrik Mistarz<sup>2</sup>; Alexander Schwahn<sup>3</sup>; Fiona Rupprecht<sup>4</sup>; <sup>1</sup>*Thermo Fisher Scientific, Morpeth, United Kingdom*; <sup>2</sup>*Thermo Fisher Scientific, Allerød, Denmark*; <sup>3</sup>*Thermo Fisher Scientific, Reinach, Switzerland*; <sup>4</sup>*Thermo Fisher Scientific, Bremen, Germany*
- TP 543 **Characterization of oligonucleotide therapeutics on an Ultra-High Mass Range Hybrid Quadrupole-Orbitrap Mass Spectrometer;** Kristina Szrentic<sup>1</sup>; Robert L Ross<sup>2</sup>; Andrew Norris<sup>1</sup>; Alexander Boris Schwahn<sup>1</sup>; Ales Holfeld<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Reinach, Switzerland*; <sup>2</sup>*Thermo Fisher Scientific, Lexington, MA*
- TP 544 **A data-independent acquisition mass spectrometry workflow for characterizing mRNA therapeutics;** Hiroshi Nakayama<sup>1</sup>; Masami Koike<sup>1</sup>; Yuko Nobe<sup>2</sup>; Yoshiki Nagashima<sup>3</sup>; Daisuke Higo<sup>3</sup>; Masato Taoka<sup>2</sup>; <sup>1</sup>*RIKEN Center for Sustainable Resource Science, Wako, Japan*; <sup>2</sup>*Tokyo Metropolitan University, Hachioji, Japan*; <sup>3</sup>*ThermoFisher Scientific, Yokohama, Japan*
- TP 545 **SynONIM: A synthetic nucleic acid and oligonucleotide impurity and modifications database to facilitate information sharing and facilitate MS data processing;** Jennifer L Lippens<sup>1</sup>; Biancamaria Florenzi<sup>2</sup>; Katyeny Manuela Da Silva<sup>1</sup>; Thomas Neefs<sup>1</sup>; Youzhong Liu<sup>1</sup>; Nicolas Sauwen<sup>2</sup>; Thomas De Vijlder<sup>1</sup>; <sup>1</sup>*Janssen Pharmaceutica NV, Beerse, Belgium*; <sup>2</sup>*Open Analytics, Antwerpen, Belgium*
- TP 546 **A Fully Automated Data Workflow for Quality Monitoring of Oligonucleotide Therapeutics;** YAARUB MUSA<sup>1</sup>; Catherine Evans<sup>1</sup>; Aude Tartiere<sup>2</sup>; Can Cui<sup>3</sup>; Stephen Kok<sup>2</sup>; Arnd Brandenburg<sup>1</sup>; <sup>1</sup>*Genedata AG, Basel, Switzerland*; <sup>2</sup>*Genedata Inc, San Francisco, CA*; <sup>3</sup>*Genedata Inc., Lexington, Massachusetts*
- TP 547 **NASEWEIS: a fast web-service for the analysis of Oligonucleotide modifications;** Samuel P Wein<sup>1</sup>; Oliver Kohlbacher<sup>1</sup>; <sup>1</sup>*University of Tübingen, Tübingen, Germany*
- TP 548 **Alkylimidazolium labeling of oligonucleotides improves electrospray ionization efficiencies to enable characterization of ribosomal RNA in neurons;** Max Sharin<sup>1</sup>; Kevin D Clark<sup>1</sup>; <sup>1</sup>*Tufts University, Medford, MA*
- TP 549 **Prediction of Collision-Induced Dissociation Spectra of Deprotonated Oligonucleotides;** Zhongqi Zhang<sup>1</sup>; Jason L. Richardson<sup>1</sup>; <sup>1</sup>*Amgen Inc., Thousand Oaks, CA*
- TP 550 **Oligonucleotides characterization using single quadrupole mass spectrometer for quality control;** Udara Jayasundara<sup>1</sup>; Vikki Johnson<sup>1</sup>; Stephen Kurzyniec<sup>1</sup>; Evelyn Wang<sup>2</sup>; Yoshiyuki Okamura<sup>2</sup>; <sup>1</sup>*Shimadzu scientific instruments, Carlsbad, CA*; <sup>2</sup>*Shimadzu Scientific Instruments, Columbia, MD*
- TP 551 **Computer Modeling of the Effectiveness of MS1 and MS2 for RNA Sequence Confirmation;** Clara Bern<sup>1</sup>; Maria Basanta-Sanchez<sup>2</sup>; Steven Broome<sup>2</sup>; Ignat Shilov<sup>2</sup>; Wilfred Tang<sup>2</sup>; Marshall W. Bern<sup>2</sup>; <sup>1</sup>*Carlmont High School, Belmont, CA*; <sup>2</sup>*Protein Metrics, LLC, Cupertino, CA*
- TP 552 **Investigations in LC/MS and LC/UV Analysis of Very Large Intact Oligonucleotides Using Various IP-RP Mobile Phases and Column Chemistries;** Sujatha Chilakala<sup>1</sup>; Roxana Eggleston-Rangel<sup>1</sup>; Michael McGinley<sup>1</sup>; Helen Harrington<sup>2</sup>; <sup>1</sup>*Phenomenex, Torrance, CA*; <sup>2</sup>*Phenomenex, London, United Kingdom*
- TP 553 **RNA identification using Zn2+/Tris catalyzed hydrolysis and liquid chromatography-mass spectrometry;** Audriv Jebe<sup>1, 2, 3, 4</sup>; Raobo XU<sup>1, 2, 3, 4</sup>; Liqing He<sup>1, 2, 3, 4</sup>; Xipeng Ma<sup>1, 2, 3, 4</sup>; Eugene G. Mueller<sup>1</sup>; Craig J. McClain<sup>1, 2, 4, 5, 6</sup>; Xiang Zhang<sup>1, 2, 3, 4, 6</sup>; <sup>1</sup>*University of Louisville, Louisville, KY*; <sup>2</sup>*University of Louisville Hepatobiology & Toxicology Center of Biomedical Research Excellence, Louisville, KY*; <sup>3</sup>*University of Louisville Alcohol Research Center, Louisville, KY*; <sup>4</sup>*Center for Regulatory and Environmental Analytical Metabolomics, Louisville, KY*; <sup>5</sup>*Department of Medicine, Louisville, KY*; <sup>6</sup>*Department of Pharmacology and Toxicology, University of Louisville, Louisville, KY*
- TP 554 **Ultra-sensitive quantitation of therapeutic oligonucleotide in human plasma by a high resolution accurate mass Orbitrap mass spectrometer;** Hao Yang<sup>1</sup>; Min Du<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Lexington, MA*
- TP 555 **Identification of HELLS as a Novel G-quadruplex Helicase;** Zi Gao<sup>1</sup>; Xiaomei He<sup>1</sup>; Yie Woon Chong<sup>1</sup>; Jun

## TUESDAY POSTERS

- Yuan<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- TP 556 **A Novel and Highly Effective LC/MS Method for Phosphorodiamidate Morpholino Oligomer (PMO) Impurity and Sequencing Analysis;** Guannan Li<sup>1</sup>; Peter Rye<sup>2</sup>; Vincent Guerlavais<sup>3</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Agilent Technologies, Lexington, MA; <sup>3</sup>Sarepta Therapeutics, Cambridge, MA
- TP 557 **Oligonucleotide Workflow Incorporating Nuclease-Conjugated Beads with LC-MS/MS;** Shweta Chhajed<sup>1</sup>; William M. McGee<sup>1</sup>; Robert Ross<sup>1</sup>; Voin Petrović<sup>2</sup>; Axl Alois Neurauter<sup>2</sup>; Dave Odelson<sup>1</sup>; James L. Stephenson Jr<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Lexington, MA; <sup>2</sup>Thermo Fisher Scientific, Oslo, Norway
- PEPTIDOMICS AND IMMUNOPEPTIDOMICS**  
**558-587**
- TP 558 **Dia-PASEF for in-depth immunopeptidomics analysis: Challenges and new opportunities;** Kristina Marx<sup>1</sup>; Naomi Hoenisch Gravel<sup>2, 3</sup>; Juliane Walz<sup>3, 4, 5, 6</sup>; Pierre-Olivier Schmit<sup>7</sup>; Torsten Mueller<sup>1</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>2</sup>Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tuebingen, Tuebingen, Germany; <sup>3</sup>Cluster of Excellence iFIT (ECX2180) "Image-Guided and Functionally Instructed Tumor Therapies"; University of Tuebingen, Tuebingen, Germany; <sup>4</sup>Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tuebingen, Tuebingen, Germany; <sup>5</sup>Clinical Collaboration Unit Translational Immunology, Department of Internal Medicine, University Hospital Tuebingen, Tuebingen, Germany; <sup>6</sup>German Cancer Research Consortium (DKTK) and German Cancer Research Center (DKFZ), partner site Tuebingen, Tuebingen, Germany; <sup>7</sup>Bruker France SAS, Wissembourg, France
- TP 559 **Investigating the Impact of Copper Toxicity on Antimicrobial Peptides in *Callinectes sapidus*: A Mass Spectrometry Approach to Hemolymph and Hemocytes;** Tina C Dang<sup>1</sup>; Wenxin Wu<sup>2</sup>; Lingjun Li<sup>1, 2</sup>; <sup>1</sup>University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin; <sup>2</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, WI
- TP 560 **Alterations in Neuropeptide Distribution in Stomatogastric Nervous System of Blue Crab *Callinectes sapidus* Under Hypoxia;** Thao U Duong<sup>1</sup>; Penghsuan Huang<sup>1</sup>; Ashley Phetsanthad<sup>1</sup>; Vu Ngoc Huong Tran<sup>2</sup>; Lingjun Li<sup>1, 2</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, WI; <sup>2</sup>University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin
- TP 561 **Quantitative Assessment of Feeding-Induced Neuropeptidome Changes via Multiplexed Mass Spectrometry;** Mitchell Gray<sup>1</sup>; Lauren Fields<sup>1</sup>; Tina C Dang<sup>2</sup>; Angel E Ibarra<sup>1</sup>; Wenxin Wu<sup>1</sup>; Lingjun Li<sup>1, 2</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin; <sup>2</sup>University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin
- TP 562 **Neuropeptide Secretion in Crustacean in Response to Feeding via In vivo Microdialysis;** Vu Ngoc Huong Tran<sup>1</sup>; Gaoyuan Lu<sup>1</sup>; Thao U Duong<sup>2</sup>; Zachary P Del Mundo<sup>1</sup>; Lingjun Li<sup>1, 2</sup>; <sup>1</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- TP 563 **Circadian changes in the cerebrospinal fluid peptidome & proteome found by nanoLC-IMS-QqTOF;** Shannon D Berneche<sup>1, 2</sup>; Sarah Asif<sup>2</sup>; Wei-Chun Kao<sup>2</sup>; Taylor Jorgensen<sup>2</sup>; Dharmeshkumar Parmar<sup>3</sup>; Martha U Gillette<sup>2, 4</sup>; Jonathan V Sweedler<sup>2, 3</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign, Urbana, IL; <sup>2</sup>Neuroscience Program, University of Illinois Urbana-Champaign, Urbana, IL; <sup>3</sup>Department of Chemistry, University of Illinois Urbana-Champaign, Champaign, IL; <sup>4</sup>Department of Cell and Developmental Biology, University of Illinois Urbana-Champaign, Urbana, IL
- TP 564 **In-silico library and two-step search improve data-independent acquisition immunopeptidomics;** Yuanliang Zhang<sup>1</sup>; Lei Chen<sup>1</sup>; Qian Zhao<sup>1</sup>; <sup>1</sup>The Hong Kong Polytechnic University, Hong Kong, Hong Kong
- TP 565 **Advancing Clinical Peptidome Profiling in Plasma with a Robust High-Throughput Workflow;** Andreas Zellner<sup>1</sup>; Steffen Tiedt<sup>2</sup>; Chien-Yun Lee<sup>1</sup>; <sup>1</sup>Technical University of Munich (TUM), Freising, Germany; <sup>2</sup>Ludwig-Maximilians-University of Munich (LMU), Munich, Germany
- TP 566 **An AI-driven, proteogenomics-based and complete workflow for novel neoantigen discovery;** Qing Zhang<sup>1</sup>; Kyle Hoffman<sup>1</sup>; Sahar Rabinoviz<sup>1</sup>; Chao Peng<sup>2</sup>; Lei Xin<sup>1</sup>; Baozhen Shan<sup>1</sup>; <sup>1</sup>Bioinformatics Solutions Inc, Waterloo, ON; <sup>2</sup>BaizhenBio Inc., Wuhan, China
- TP 567 **Using targeted mass spectrometry to characterize the mechanism of action for a novel T cell-priming vaccine delivery system;** Richard Brase<sup>1</sup>; Hager Mohamed<sup>1</sup>; Aykan Karabudak<sup>1</sup>; Xiaofang Huang<sup>1</sup>; <sup>1</sup>Emergex Vaccines, Doylestown, PA
- TP 568 **Streamlined LC/MS methods to quantitate MHC-I peptides in the development of neoantigen-directed therapeutics;** Arun Tailor<sup>1</sup>; Jason LaMar<sup>1</sup>; Alisa Arata<sup>1</sup>; Sebastian Guelman<sup>1</sup>; Surinder Kaur<sup>1</sup>; Ola M Saad<sup>1</sup>; <sup>1</sup>Department of BioAnalytical Sciences, Genentech, Inc., South San Francisco, California
- TP 569 **Total HLA Class II Quantification in Dendritic Cells (DCs) to Complement MHC Associated Peptide Proteomics (MAPPs) for Immunogenicity Risk Assessment;** Jason LaMar<sup>1</sup>; Alisa Arata<sup>2</sup>; Violet Lee<sup>2</sup>; Arun Tailor<sup>2</sup>; Sylvia Wong<sup>2</sup>; Surinder Kaur<sup>2</sup>; Ola M Saad<sup>2</sup>; <sup>1</sup>Genentech - South San Francisco, CA, South San Francisco, CA; <sup>2</sup>Genentech Inc, South San Francisco, CA
- TP 570 **Maximizing immunopeptide identification and reproducibility from minute pediatric solid tumor biopsy samples;** Peiyao Li<sup>1</sup>; Richa Kapoor<sup>1</sup>; John M. Maris<sup>1, 2</sup>; Diego Assis<sup>3</sup>; Matthew Willetts<sup>3</sup>; Hossein Fazelinia<sup>1</sup>; Lynn A Spruce<sup>1</sup>; <sup>1</sup>Children's Hospital of Philadelphia, Philadelphia, PA; <sup>2</sup>University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; <sup>3</sup>Bruker Scientific, LLC, Billerica, MA
- TP 571 **ImmunoResource: Noncanonical MHC-I associated peptide database compounded by proteogenomic analysis of immunopeptidome data;** Yoonwoo Lee<sup>1</sup>; Seunghyuk Choi<sup>2</sup>; Eunok Paik<sup>1, 2</sup>; <sup>1</sup>Department of Artificial Intelligence, Hanyang University, Seoul, South Korea; <sup>2</sup>Department of Computer Science, Hanyang University, Seoul, South Korea
- TP 572 **Towards a comprehensive panMHC-II MAPPs (MHC-II Associated Peptide Proteomics) analysis to assess immunogenicity risks of biotherapeutics;** Axel Ducret<sup>1</sup>; Maureen Bardet<sup>1</sup>; Shahrzad Tavalei<sup>1</sup>; Katharina Hartman<sup>1</sup>; Céline Marban-Doran<sup>1</sup>; <sup>1</sup>Roche Innovation Center Basel (RICB), Switzerland, Switzerland
- TP 573 **Development of a novel high-sensitivity peptidomics platform based on capillary electrophoresis coupled with a high-resolution mass spectrometry;** Tomooki Nitta<sup>1</sup>; Kazunori Sasaki<sup>1</sup>; Hiroyuki Yamamoto<sup>1</sup>; Kenjiro Kami<sup>1</sup>; <sup>1</sup>Human Metabolome Technologies, Inc., Tsuruoka, Japan
- TP 574 **TIMSrescore: timsTOF-optimized PSM rescoring boosts identification rates for immunopeptidomics;** Arthur Declercq<sup>1</sup>; Jonathan Krieger<sup>2</sup>; George Rosenberger<sup>3</sup>; Ralf Gabriels<sup>1</sup>; Robbin Bouwmeester<sup>1</sup>; Tharan Srikumar<sup>2</sup>; Sven Degroeve<sup>1</sup>; Dennis Tredé<sup>4</sup>; Lennart Martens<sup>1</sup>; <sup>1</sup>VIB-UGent Center for Medical Biotechnology, Gent, Belgium; <sup>2</sup>Bruker Ltd., Milton, ON; <sup>3</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>4</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- TP 575 **Abemaciclib differentially affects the immunopeptidome of breast cancer subtypes;** Robin Minati<sup>1, 2</sup>; Eralda Kina<sup>1, 2</sup>; Eric Bonneil<sup>1</sup>; Joel Lanoix<sup>1</sup>; Marie-Pierre Hardy<sup>1</sup>; Krystel Vincent<sup>1</sup>; Claude Perreault<sup>1, 3</sup>; Pierre Thibault<sup>1, 4</sup>; <sup>1</sup>Institute of

## TUESDAY POSTERS

- Research in Immunology and Cancer, Université de Montréal, Montreal, QC; <sup>2</sup>Molecular biology program, Université de Montréal, Montréal, QC; <sup>3</sup>Department of Medicine, Université de Montréal, Montreal, QC; <sup>4</sup>Department of Chemistry, Université de Montréal, Montréal, QC
- TP 576 **Distinguishing MIPs in the cell surface or in processing by MS with immunoprecipitation and Mild Acid Elution methods;** Chao Peng<sup>1</sup>; Ping Wu<sup>1</sup>; Haofei Miao<sup>1</sup>; Ling Li<sup>1</sup>; Baozhen Shan<sup>1</sup>; <sup>1</sup>BaizhenBio Inc., Wuhan, China
- TP 577 **Advanced Immunopeptidomics Pipeline Unveils Significantly Expanded Noncanonical Neoantigen Repertoire Following Spliceosome Perturbation;** Jongmin Choi<sup>1</sup>; Seunghyuk Choi<sup>1</sup>; Elizabeth A. Bowling<sup>1</sup>; Matthew V. Holt<sup>1</sup>; Kristen L. Karlin<sup>1</sup>; Matthew Willetts<sup>2</sup>; Ruben Shrestha<sup>2</sup>; Diego Assis<sup>2</sup>; Jarey H. Wang<sup>1</sup>; Sara J. Wright<sup>1</sup>; Adithya Balasubramanian<sup>1</sup>; Hyun-Sung Lee<sup>1</sup>; Thomas Westbrook<sup>1</sup>; Bing Zhang<sup>1</sup>; <sup>1</sup>Baylor College of Medicine, Houston, TX; <sup>2</sup>Bruker life sciences, Billerica, MA
- TP 578 **No enzyme? No problem! An accessible, scalable multi-omic cloud-based solution for efficient MS-based endogenous peptidomics and immunopeptidomics;** Reid Wagner<sup>1,2</sup>; James E Johnson<sup>1,2</sup>; Subina Mehta<sup>1</sup>; Kyle Richards<sup>1</sup>; Suzanne Coleman<sup>1</sup>; David A Largaespada<sup>1</sup>; Monica E Kruk<sup>1</sup>; Chris H Wendt<sup>1,3</sup>; Bing Zhang<sup>4</sup>; Fengchao Yu<sup>5</sup>; Alexey I Nesvizhskii<sup>6</sup>; Pratik D. Jagtap<sup>1</sup>; Tim Griffin<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>Minnesota Supercomputing Institute, Minneapolis, MN; <sup>3</sup>Minneapolis VA Health Care System, Minneapolis, MN; <sup>4</sup>Baylor College of Medicine, Houston, Texas; <sup>5</sup>University of Michigan, Ann Arbor, Michigan
- TP 579 **Trapped ion mobility-coupled mass spectrometry reveals high frequent tumor-associated antigens in chronic lymphocytic leukemia;** Naomi Hoenisch Gravel<sup>1,2</sup>; Jonas Scheid<sup>1,2,3</sup>; Marcel Wacker<sup>1,2</sup>; Yacine Maringer<sup>1,2</sup>; Jens Bauer<sup>1,2</sup>; Juliane Walz<sup>1,2,4,5</sup>; <sup>1</sup>Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tuebingen, Tuebingen, Germany; <sup>2</sup>Cluster of Excellence iFIT (EXC2180) "Image-Guided and Functionally Instructed Tumor Therapies"; University of Tuebingen, Tuebingen, Germany; <sup>3</sup>Quantitative Biology Center QBIC, University of Tuebingen, Tuebingen, Germany; <sup>4</sup>Clinical Collaboration Unit Translational Immunology, Department of Internal Medicine, University Hospital Tuebingen, Tuebingen, Germany; <sup>5</sup>German Cancer Consortium (DKTK) and German Cancer Research Center (DKFZ), partner site Tuebingen, Tuebingen, Germany
- TP 580 **Advancing Low input Chromatography: Developing a novel Column for Improved Immunopeptidomics IDs;** Benoit Fatou<sup>1</sup>; Michael Krawitzky<sup>2,3</sup>; Ruben Shrestha<sup>4</sup>; Diego Assis<sup>5</sup>; Nicholas Cheung<sup>6</sup>; Darshit Shah<sup>6</sup>; Robert Salzler<sup>6</sup>; Matthew Willetts<sup>7</sup>; <sup>1</sup>Bruker Scientific, LLC, Billerica, MA; <sup>2</sup>Bruker Daltonics, San Jose, CA; <sup>3</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>4</sup>Bruker Scientific LLC, San Jose, CA; <sup>5</sup>Bruker Scientific, Billerica, MA; <sup>6</sup>Regeneron Pharmaceuticals, Tarrytown, NY; <sup>7</sup>Bruker Daltonics GmbH & Co. KG, Billerica, MA
- TP 581 **Assessing a Single Mutation's Effect on Immunogenicity of FLT3L-Fc;** Qui Phung<sup>1</sup>; Yinyin Li<sup>1</sup>; Zhenru Zhou<sup>1</sup>; Sivan Cohen<sup>1</sup>; Travis Bainbridge<sup>1</sup>; Mercedesz Balazs<sup>1</sup>; Jennie Lill<sup>1</sup>; Dan Qin<sup>1</sup>; <sup>1</sup>Genentech Inc, South San Francisco, CA
- TP 582 **Mhcquant enables scalable and reproducible immunopeptidomics analyses with enhanced peptide identification using streamlined peptide property predictors;** Jonas Scheid<sup>1,2,3</sup>; Steffen Lemke<sup>1,2,3</sup>; Naomi Hoenisch Gravel<sup>1,2</sup>; Timo Sachsenberg<sup>4,5</sup>; Arthur Declercq<sup>6</sup>; Ralf Gabriels<sup>6,7</sup>; Jens Bauer<sup>1,2</sup>; Leon Bichmann<sup>8</sup>; Marissa Lisa Dubbelaar<sup>1,2,3</sup>; Juliane Sarah Walz<sup>1,2,9,10</sup>; Sven Nahnsen<sup>3,11</sup>; <sup>1</sup>Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tuebingen, Tuebingen, Germany; <sup>2</sup>Cluster of Excellence iFIT (EXC2180) "Image-Guided and Functionally Instructed Tumor Therapies", University of Tuebingen, Tuebingen, Germany; <sup>3</sup>Quantitative Biology Center (QBIC), University of Tuebingen, Tuebingen, Germany; <sup>4</sup>Institute for Bioinformatics and Medical Informatics, University of Tuebingen, Tuebingen, Germany; <sup>5</sup>Applied Bioinformatics, Department of Computer Science, University of Tuebingen, Tuebingen, Germany; <sup>6</sup>VIB-UGent Center for Medical Biotechnology, VIB, Ghent, Belgium; <sup>7</sup>Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; <sup>8</sup>Center for Systems and Engineering Immunology (CSEI), School of Medicine, Yale University, New Haven, CT; <sup>9</sup>Clinical Collaboration Unit Translational Immunology, Department of Internal Medicine, University Hospital Tuebingen, Tuebingen, Germany; <sup>10</sup>German Cancer Consortium (DKTK) and German Cancer Research Center (DKFZ), partner site Tuebingen, Tuebingen, Germany; <sup>11</sup>Department for Computer Science, Biomedical Data Science, University of Tuebingen, Tuebingen, Germany
- TP 583 **Discovering physiological substrates for the coronavirus host receptor protease ACE2 using stable isotope signature labeling;** Fabian Schulte<sup>1</sup>; Markus Hardt<sup>1</sup>; <sup>1</sup>Forsyth Institute, Cambridge, MA
- TP 584 **Thunder-DDA-PASEF boosted by MS2Rescore enables high sensitivity and high-coverage immunopeptidomics;** David Gomez-Zepeda<sup>1,2</sup>; Danielle Arnold-Schild<sup>3</sup>; Julian Beyrle<sup>1,2</sup>; Arthur Declercq<sup>4,5</sup>; Ralf Gabriels<sup>4,5</sup>; Annica Preikschat<sup>3</sup>; Mateusz Lacki<sup>3</sup>; Aurélie Hirschler<sup>6</sup>; Jeewan Babu Rial<sup>6</sup>; Christine Carapito<sup>6</sup>; Lennart Martens<sup>4,5</sup>; Ute Distler<sup>3</sup>; Hansjörg Schild<sup>3</sup>; Stefan Tenzer<sup>1,2,3</sup>; <sup>1</sup>Helmholtz Institute for Translational Oncology Mainz (HITRON Mainz) – A Helmholtz Institute of the DKFZ, Mainz, Germany; <sup>2</sup>DKFZ German Cancer Research Center, Heidelberg, Germany; <sup>3</sup>University Medical Center Mainz, Mainz, Germany; <sup>4</sup>VIB - UGent Center for Medical Biotechnology, Ghent, Belgium; <sup>5</sup>Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; <sup>6</sup>BioOrganic Mass Spectrometry Laboratory (LSMBO), IPHC UMR 7178, University of Strasbourg, CNRS, ProFI, Strasbourg, France
- TP 585 **A Semi-Targeted Orbitrap Tribrid Method for Simultaneous Quantification and Discovery of Immunopeptides;** David Bergen<sup>1</sup>; Lilian R Heil<sup>1</sup>; Jingjing Huang<sup>1</sup>; Tonya Pekar Hart<sup>1</sup>; Rafael Melani<sup>1</sup>; Vlad Zabrouskov<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA
- TP 586 **Immunopeptidomic landscape of non-small cell lung carcinoma;** Kiran K. Mangalaparthi<sup>1</sup>; Partho S. Sen<sup>1</sup>; Richard K. Kandasamy<sup>1</sup>; Aaron S. Mansfield<sup>2</sup>; Akhilesh Pandey<sup>1,3</sup>; <sup>1</sup>Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, MN 55905; <sup>2</sup>Department of Oncology, Mayo Clinic, Rochester, MN 55905; <sup>3</sup>Center for Individualized Medicine, Mayo Clinic, Rochester, MN 55905
- TP 587 **Predicting effectively complete immunopeptidome spectral libraries to improve the detection of neoantigens;** Lewis Geer<sup>1</sup>; Douglas Slotta<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD

### PHOSPHOPEPTIDES AND PHOSPHOPROTEINS 588-608

- TP 588 **Proteomics and Phosphoproteomics Reveals Unique Alterations in KRAS and P53 Mutant Colorectal Cancer Spheroids after Fatty Acid Synthase Inhibition;** Brian D Fries<sup>1</sup>; Amanda B Hummon<sup>1,2</sup>; <sup>1</sup>The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; <sup>2</sup>Comprehensive Cancer Center, Columbus, OH
- TP 589 **Towards high-dimensional phosphoproteomics with data-independent acquisition and μPhos;** Denys Oliinyk<sup>1</sup>; Ilka Klose<sup>1</sup>; Dilfuza Ernafasova<sup>1</sup>; Felix Schneidmadel<sup>1</sup>; Florian Meier<sup>1</sup>; <sup>1</sup>University Klinikum Jena, Jena, Germany
- TP 590 **Phosphoproteomic analysis of low-input FFPE tissue samples with DIA-MS method;** Stephanie Zalesak-Kravec<sup>1</sup>; Yeoun Jin Kim<sup>1</sup>; David J Clark<sup>1</sup>; <sup>1</sup>AstraZeneca, Gaithersburg, MD

## TUESDAY POSTERS

- TP 591 **Systematic optimization of automated phosphopeptide enrichment for high-sensitivity phosphoproteomics;** Patricia Bortel<sup>1</sup>; Ilaria Piga<sup>2</sup>; Claire Koenig<sup>2</sup>; Christopher Gerner<sup>1</sup>; Ana Martinez-Val<sup>2, 3</sup>; Jesper Velgaard Olsen<sup>2</sup>; <sup>1</sup>Department of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria; <sup>2</sup>Novo Nordisk Foundation Center for Protein Research, Proteomics Program, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; <sup>3</sup>Centro Nacional de Investigaciones Cardiovasculares Carlos III (CNIC), Madrid, Spain
- TP 592 **High throughput semi-automated platform for the identification of post-translational modifications (PTMs) specific biomarkers from plasma samples;** Santosh D. Bhosale<sup>1</sup>; Angel Keoseyan<sup>1</sup>; Josselin Ortiz<sup>1</sup>; Nathan Hendricks<sup>1</sup>; Annie Moradian<sup>1</sup>; Susan M. Mockus<sup>1</sup>; <sup>1</sup>Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA
- TP 593 **Dissecting the Temporal Dephosphorylation of DNA Damage Response Proteins by SPN-PP1 using DIA Phospho-proteomics;** Mi Young Son<sup>1</sup>; Minkyu Kim<sup>1</sup>; <sup>1</sup>UT Health Science Center at San Antonio, San Antonio, TX
- TP 594 **IMAC-enabled Phosphoproteomic Analysis of pLRRK2, pRab10 and pRab12 in Mouse Tissues;** Junpeng Xiao<sup>1</sup>; Caitlyn Keck<sup>1</sup>; David B Shaw<sup>1</sup>; Nil Tandogan-Grey<sup>1</sup>; Paresh Sanghani<sup>1</sup>; Theresa A Day<sup>1</sup>; Michael Chalmers<sup>1</sup>; <sup>1</sup>Eli Lilly & Company, Indianapolis, IN
- TP 595 **Development of mass spectrometry-based methods to identify C-terminal tail residues in the Glucagon receptor that are phosphorylated following agonism;** Ian Michael Lamb<sup>1</sup>; Alex D White<sup>1</sup>; Francis S Willard<sup>1</sup>; Michael J Chalmers<sup>1</sup>; Junpeng Xiao<sup>1</sup>; <sup>1</sup>Eli Lilly & Company, Indianapolis, IN
- TP 596 **SmartPhos: Streamlining High-Throughput, Low-input Phosphoproteomics for Dynamic Cellular Insights;** Barbara Helm<sup>1, 2</sup>; Dario Frey<sup>1, 2</sup>; Cong Quan Ta<sup>1</sup>; Yueyang Xie<sup>1</sup>; Shubham Agrawal<sup>3</sup>; Marcel Schilling<sup>1</sup>; Junyan Lu<sup>3</sup>; Ursula Klingmüller<sup>1, 2</sup>; <sup>1</sup>Division Systems Biology of Signal Transduction, German Cancer Research Center (DKFZ), Heidelberg, Germany; <sup>2</sup>German Center for Lung Research (DZL) and Translational Lung Research Center Heidelberg (TRLG), Heidelberg, Germany; <sup>3</sup>Computational Omics and Precision Oncology, Heidelberg University, Faculty of Medicine, Heidelberg University Hospital, Heidelberg, Germany
- TP 597 **Quantitative Global Proteome and Phosphoproteome Analysis of Caenorhabditis elegans Embryos Utilizing a FAIMS-based DIA Platform.;** Colt D Capan<sup>1</sup>; Michael P Vincent<sup>1</sup>; Jason Copper<sup>1</sup>; Ibukunoluwa Sodiya<sup>1</sup>; Nick Burton<sup>1</sup>; Ryan D Sheldon<sup>1</sup>; Hyoungjoo Lee<sup>1</sup>; <sup>1</sup>Van Andel Institute, Grand Rapids, MI
- TP 598 **Advancing qualitative phosphoproteomics via the integration of FAIMS and non-FAIMS analysis;** Byoung-Kyu Cho<sup>1</sup>; Young Ah Goo<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO
- TP 599 **SARS-CoV-2 Virion Proteomics Revealed Protein Phosphatase-1;** Jyothirmai Simhadri<sup>1</sup>; Philipp A Illyin<sup>2, 3</sup>; Kai Huang<sup>2, 3</sup>; Andrey Ivanov<sup>1</sup>; Xionghao Lin<sup>1</sup>; Tatiana Ammosova<sup>1, 4</sup>; Alexander Bukreyev<sup>2, 3</sup>; Sergei Nekhai<sup>1, 4</sup>; <sup>1</sup>Center for Sickle Cell Disease, Howard University, Washington, DC; <sup>2</sup>Department of Pathology, University of Texas Medical Branch, Galveston, TX; <sup>3</sup>Galveston National Laboratory, Galveston, TX; <sup>4</sup>Department of Medicine, College of Medicine, Howard University, Washington, DC
- TP 600 **Chemoproteomic mapping of aldehyde-containing metabolite interactome by mass spectrometry;** Juhee Park<sup>1, 2</sup>; Jong-Seo Kim<sup>1, 2</sup>; <sup>1</sup>School of Biological Sciences, Seoul National University, Seoul, South Korea; <sup>2</sup>Center for RNA Research, Institute of Basic Science (IBS), Seoul, South Korea
- TP 601 **Comprehensive phosphoproteomic analysis using integrated IMAC and antibody-based phosphopeptide enrichment and mass spectrometry;** Liyuan Jiao<sup>1</sup>; T. Mamie Lih<sup>1</sup>; Lijun Chen<sup>1</sup>; Yuefan Wang<sup>1</sup>; Jongmin Woo<sup>1</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- TP 602 **Classification of mass spectrometry-identified phosphosites unravels potential new functions of the unannotated phosphoproteome;** Pedro R. Cutillas; <sup>1</sup>Queen Mary University of London, London, United Kingdom
- TP 603 **A fine-tune optimization of phosphoproteomics DIA analysis for a more robust and insightful candidate selection;** Sara Ceccacci<sup>1</sup>; Cerina Chhuon<sup>1</sup>; Kevin Roger<sup>1</sup>; Ines Metatla<sup>1</sup>; Joanna Lipecka<sup>1</sup>; Chiara Guerrera<sup>1</sup>; <sup>1</sup>Necker Proteomics Platform, INSERM US24, Paris, France
- TP 604 **Evaluation of phosphopeptide enrichment using different metal ions for sensitive nano-scale phosphoproteomics;** Hyeyoon Kim<sup>1</sup>; Marina A Gritsenko<sup>2</sup>; Vanessa Paurus<sup>2</sup>; Reta Birhanu Kitata<sup>2</sup>; Ronald J. Moore<sup>2</sup>; Rosalie K. Chu<sup>3</sup>; Karl K. Weitz<sup>2</sup>; Tao Liu<sup>2</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>3</sup>Pacific Northwest National Lab, Richland, WA
- TP 605 **Top-down characterization of genetically encoded Bcl-XL phosphorylation and phosphomimetics using electron capture dissociation;** Rachel Franklin<sup>1</sup>; Cat Hoang Vesely<sup>2</sup>; Richard B. Cooley<sup>2</sup>; Joseph Meeuswen<sup>1</sup>; <sup>1</sup>Agilent Technologies, Corvallis, Oregon; <sup>2</sup>Oregon State University- GCE4ALL Center, Corvallis, Oregon
- TP 606 **Phospho-signaling regulatory mechanisms driving beta cell insulin secretion;** Mohammad Ovais Azizzaniani<sup>1</sup>; Rachel Elizabeth Turn<sup>1</sup>; Anushweta Asthana<sup>1</sup>; Artemis Xu<sup>1</sup>; Peter K. Jackson<sup>1</sup>; <sup>1</sup>Jackson Laboratory, Baxter Laboratory for Stem Cell Biology, Department of Microbiology & Immunology, Stanford University School of Medicine, Stanford, CA
- TP 607 **RUPE-phospho : Rapid ultrasound-assisted peptide-identification-enhanced phosphoproteomics workflow for microscale samples;** Dongxue Wang; <sup>1</sup>Beijing Proteome Research Center, National Center for Protein Sciences, Beijing, China; The  $\pi$ -HuB Project Infrastructure, Guangzhou, China; International Institute for Phronesis Medicine, Guangzhou, China; South China Institute of Biomedicine, Guangzhou, China
- TP 608 **Benchmarking Orbitrap Fusion Lumos TMT quantitation versus Orbitrap Astral LFQ data independent acquisition (DIA) mass spectrometry for phosphoproteome analysis;** Gregory K Potts<sup>1</sup>; Shaun McLoughlin<sup>2</sup>; Janice Y Lee<sup>2</sup>; Hua Tang<sup>2</sup>; Jon D Williams<sup>2</sup>; Scott E Warder<sup>2</sup>; <sup>1</sup>AbbVie, Inc., North Chicago, IL; <sup>2</sup>AbbVie Inc., North Chicago, IL

### PLANT BIOLOGY AND BIOTECHNOLOGY 609-620

- TP 609 **Characterisation of stress response at the proteome and transcriptome level in rice under a range of abiotic stress conditions;** Fatemeh Habibpourmehraban<sup>1</sup>; Zahra Ghorbanzadeh<sup>2</sup>; Farhad Masoomi-Aladizgeh<sup>1</sup>; Yunqi Wu<sup>1</sup>; Sara Hamzelou<sup>1</sup>; Dylan Multari<sup>1</sup>; Ardeshir Amirkhani<sup>1</sup>; Mehdi Mirzaei<sup>1</sup>; Ghasem Hosseini Salekdeh<sup>1</sup>; Mohammad Reza Ghaffari<sup>2</sup>; Brian J. Atwell<sup>1</sup>; Paul A. Haynes<sup>1</sup>; <sup>1</sup>Macquarie University, North Ryde, Australia; <sup>2</sup>Department of Systems Biology, Agricultural Biotechnology Research Institute of Iran (ABRII), Karaj, Iran
- TP 610 **Identification of Compounds Present in the Endangered Plant Ziziphus celata: Both Host and Endophyte Origins;** Kate Calvin<sup>1</sup>; Kim Pham<sup>1</sup>; Esmeralda Morales<sup>1</sup>; Jesus Hernandez<sup>1</sup>; <sup>1</sup>South Florida State College, Avon Park, FL
- TP 611 **SPATIAL EXOMETABOLOMICS OF THE POPLAR RHIZOSPHERE GROWN IN MICROFLUIDIC SOIL-LIKE HABITATS;** Kevin J Zemaits<sup>1</sup>; Jayde Aufrecht<sup>1</sup>; Daisy Herrera<sup>1</sup>; Petrus Zwart<sup>2</sup>; Tanya Winkler<sup>1</sup>; Christopher Anderton<sup>1</sup>; Sharon Doty<sup>3</sup>; Amir Ahkami<sup>1</sup>; Dušan Veličković<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Lawrence Berkeley National Laboratory, Berkeley, CA; <sup>3</sup>University of Washington, Seattle, WA

## TUESDAY POSTERS

- TP 612 **Mass Spectrometry-based Methods for Selective Detection of Inositol Poly- and Pyrophosphates: Implications for Cellular Processes and Biological Significance;** Hector Najera-Gonzalez<sup>1</sup>; Luis Herrera-Estrella<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, Texas
- TP 613 **Large scale plant protein turnover measurement: a 15N metabolic approach in development;** Will V. Bienenvenut<sup>1</sup>; Marie-Helene Andrieux<sup>2</sup>; Oliver LANGELLA<sup>1</sup>; Thierry Balliau<sup>1</sup>; Sophie COLOMBIE<sup>2</sup>; Mélisande BLEIN-NICOLAS<sup>1</sup>; <sup>1</sup>GQE - le moulon, Gif sur Yvette, France; <sup>2</sup>Biologie du Fruit, INRAE, Bordeaux, France
- TP 614 **Widely targeted metabolomics and subsequent label-free analysis identified candidate metabolites that control hypocotyl elongation in the model plant *Arabidopsis thaliana*;** HIROMITSU TABETA<sup>1</sup>; Tetsuya Mori<sup>1</sup>; Ali Ferjani<sup>2</sup>; Masami Hirai<sup>1</sup>; <sup>1</sup>RIKEN CSRS, Yokohama, Japan; <sup>2</sup>Tokyo Gakugei University, Koganei-shi, Japan
- TP 615 **Preliminary Identification of Specialized Metabolite Secretions and Secretory Pathways in *Medicago truncatula* Border Cells;** Clayton Kranawetter<sup>1, 2, 3, 4</sup>; Lloyd W. Sumner<sup>1, 2, 3, 4</sup>; <sup>1</sup>University of Missouri-Columbia, Columbia, MO; <sup>2</sup>MU Metabolomics Center, Columbia, MO; <sup>3</sup>Christopher S. Bond Life Sciences Center, Columbia, MO; <sup>4</sup>Interdisciplinary Plant Group, Columbia, MO
- TP 616 **Distribution analysis of related substances to elucidate the function of phytoalexins in plant-pathogen interactions;** Kaoru Nakagawa<sup>1</sup>; Koji Okuda<sup>1</sup>; Eriko Betsuyaku<sup>2</sup>; Toshiya Matsubara<sup>3</sup>; Shigeyuki Betsuyaku<sup>2</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Ryukoku University, Otsu, Japan; <sup>3</sup>Shimadzu Scientific Instruments, Columbia, MD
- TP 617 **Selective precursor ion LC-MS/MS analysis of glucosinolates from food/nutraceuticals vegetal species;** Alberto Asteggiano<sup>1</sup>; Alex Africano<sup>2</sup>; Enrica Mecarelli<sup>1</sup>; Federica Dal Bello<sup>2</sup>; Claudio Medana<sup>2</sup>; <sup>1</sup>University of Turin, Torino, Italy; <sup>2</sup>University of Turin, Torino, Italy
- TP 618 **Integration of Omic Analyses Reveals Important Biomolecular Pathways in Photosynthetic Systems;** Mary S Lipton<sup>1</sup>; Kim K Hixson<sup>1</sup>; Carrie D Nicora<sup>3</sup>; Samuel O Purvine<sup>1</sup>; Kent J Bloodsworth<sup>1</sup>; Vanessa L Paurus<sup>1</sup>; Tanya E Winkler<sup>1</sup>; Nathalie Munoz<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- TP 619 **Molecular Networking Reveals Diversity of Phytohormones within a *Physalis* Diversity Panel;** Jennifer Shipp<sup>1</sup>; Daniel Ence<sup>1</sup>; Joe Rokicki<sup>1</sup>; Andrew Katz<sup>1</sup>; <sup>1</sup>Enveda Biosciences, Boulder, CO
- TP 620 **Reconfiguration of The Shimadzu TQ8040 Triple Quad and Deployment as an Atmospheric Monitoring Real-Time High-Definition Mass Spectrometer (3Q-RTHD-MS) and Applications;** Karl K. Weitz<sup>1</sup>; Bryson C. Gibbons<sup>1</sup>; Rosalie K. Chu<sup>1</sup>; James J. Moran<sup>1</sup>; Ljiljana Pasa Tolic<sup>1</sup>; Amir H. Ahkami<sup>1</sup>; Jennifer E. Kyle<sup>1</sup>; Tao Liu<sup>1</sup>; Mary S Lipton<sup>1</sup>; <sup>1</sup>Battelle Pacific Northwest National Laboratories, Richland, WA
- TP 624 **The ZenoTOF 7600 system facilitates precise determination of intact mass and identification of sequence variations in Defibrase;** Longlong Hu<sup>1</sup>; Ji Luo<sup>1</sup>; Hongxu Chen<sup>2</sup>; Lihai Guo<sup>2</sup>; <sup>1</sup>SCIEX, Shanghai, China; <sup>2</sup>SCIEX, Beijing, China
- TP 625 **Structural Analysis of Monoclonal Antibody Aggregation in Dynamic Heterogeneous Systems Using Liquid Chromatography Coupled with Flash Oxidation (LC-Fox) System;** Zhi Cheng<sup>1</sup>; Joshua S Sharp<sup>1, 2</sup>; Emily Chea<sup>1</sup>; Scot Weinberger<sup>1</sup>; <sup>1</sup>GenNext Technologies, Half Moon Bay, CA; <sup>2</sup>UNIVERSITY OF Mississippi, Oxford, MS
- TP 626 **Utilizing Click Chemistry for Advanced Analysis of Antibody Oxidation Intermediates using High-Resolution Intact Mass Spectrometry;** Yu Zhou<sup>1</sup>; Jakub Baudys<sup>1</sup>; John R Barr<sup>1</sup>; Dongxia Wang<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA
- TP 627 **Exploring structural changes of antibody-drug conjugates (ADCs) under stress by native limited proteolysis;** Xinhao Shao<sup>1</sup>; Nhat Le<sup>1</sup>; Shiyue Zhou<sup>1</sup>; Qunying Zhang<sup>1</sup>; Julie Heflin<sup>1</sup>; <sup>1</sup>Biologics Analytical R&D – LC/ABC, Biologics CMC Development, Development Sciences, AbbVie Inc., North Chicago, Illinois
- TP 628 **Mass spectrometry based approaches designed to ensure correct chain assembly of bispecific antibodies;** Vesela Encheva-Yokoya<sup>1</sup>; Bodhisattwa Saha<sup>1</sup>; Aysha Ali<sup>1</sup>; Francesca Ferlenghi<sup>1</sup>; Karina Bora<sup>1</sup>; James Graham<sup>1</sup>; Benedict Dirnberger<sup>1</sup>; <sup>1</sup>Lonza, London, United Kingdom
- TP 629 **Multi-level characterization and proteoform profiling of an intact monoclonal antibody using the ZenoTOF 7600;** Sarah Nguyen<sup>1, 2, 3</sup>; Armelle Martelet<sup>3</sup>; Séverine Clavier<sup>3</sup>; Sarah Cianféroni<sup>1, 2</sup>; Oscar Hernandez-Alba<sup>1, 2</sup>; <sup>1</sup>LSMBO (University of Strasbourg), Strasbourg, France; <sup>2</sup>Infrastructure Nationale de Protéomique ProFI – FR2048, Strasbourg, France; <sup>3</sup>Sanofi R&D, Vitry-sur-Seine, France
- TP 630 **Implementation of Mass Photometry as A Novel, Single Molecule Heightened Characterization Technique for Analysis of Diverse Biotherapeutic Modalities;** Lauren F Barnes<sup>1</sup>; Leah Wang<sup>1</sup>; Mingyue Li<sup>2</sup>; Vicky Lin<sup>2</sup>; Saurabh Singh<sup>1</sup>; Sutapa Barua<sup>2</sup>; Caitlin Wappelhorst<sup>1</sup>; Erika Jensen<sup>1</sup>; Clifford Entrican<sup>2</sup>; Daniel Ryan<sup>1</sup>; Qin Zou<sup>1</sup>; Anne Kim<sup>2</sup>; Jason Rouse<sup>2</sup>; <sup>1</sup>Pfizer Inc., Chesterfield, MO; <sup>2</sup>Pfizer Inc., Andover, MA
- TP 631 **Analytical Challenges in the Characterization of a Complex Fc Fusion Protein;** Felix Vega<sup>1</sup>; Eliza Dulalia<sup>1</sup>; Jorge Monteon<sup>1</sup>; Mary Nguyen<sup>1</sup>; <sup>1</sup>Alector, South San Francisco, CA
- TP 632 **Uncovering a novel seryl-like modification on a Histidine residue of a CHO-produced mAb;** Malgorzata Szyjka<sup>1</sup>; Ruiyi Dong<sup>1</sup>; Tom Cameron<sup>1</sup>; Mia Rushe<sup>1</sup>; Joseph Amatucci<sup>1</sup>; Heather Cooke<sup>1</sup>; Jana Dolnikova<sup>1</sup>; You Li<sup>1</sup>; Xiaofeng Yang<sup>1</sup>; <sup>1</sup>Biogen, Biologics Drug Discovery, Cambridge, MA
- TP 633 **Characterization of antibody therapeutics in early discovery;** Yuntao Zhang<sup>1</sup>; Aarti Jashnani<sup>1</sup>; Srikanth Kotapati<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb, Redwood City, CA
- TP 634 **Unveiling the Complexity of a Heavily Glycosylated Reagent Protein through Charge Detection Mass Spectrometry and other Biophysical Techniques;** Tian Tian<sup>1</sup>; Zoltan Szabo<sup>2</sup>; Nithya Srinivasan<sup>3</sup>; Dhan Bagal<sup>1</sup>; Iain D.G. Campuzano<sup>3</sup>; <sup>1</sup>Amgen, South San Francisco, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Amgen, Thousand Oaks, CA
- TP 635 **Therapeutic Protein Charge Variant Characterization with Intact Mass and Peptide Mapping Following Microgram Preparative Capillary Isoelectric Focusing Electrophoresis Fractionation;** Thomas Menneteau<sup>1</sup>; Claire Butré<sup>1</sup>; Géry Van Vynch<sup>1</sup>; Arnaud Delobel<sup>1</sup>; Marion Galaup<sup>2</sup>; Kristell Lebozec<sup>2</sup>; Laurence Talbot<sup>3</sup>; Kefei Wang<sup>4</sup>; <sup>1</sup>Quality Assistance, Thuin, Belgium; <sup>2</sup>Acticor Biotech, Paris, France; <sup>3</sup>Bio-Techne, Noyal Châtilion sur Seiche, France; <sup>4</sup>Bio-Techne, San Jose, CA
- TP 636 **Determination of the alpha-glucosidase anti-drug antibodies epitopes in Pompe disease patient plasma**

### PROTEIN THERAPEUTICS: STRUCTURAL CHARACTERIZATION 621-650

- TP 621 **Advancing the functional and structural characterization of deamidated proteoforms by novel mass spectrometry-based strategies;** Steffen Lippold<sup>1</sup>; Tilman Schlothauer<sup>2</sup>; Feng Yang<sup>1</sup>; <sup>1</sup>Genentech, Inc., South San Francisco, CA; <sup>2</sup>Roche Diagnostics GmbH, Penzberg, Germany
- TP 622 **Capturing TCR and peptide-HLA Interactions using Cross-linking Mass Spectrometry;** Thomas J Powell<sup>1</sup>; Vijaykumar Karupiah<sup>1</sup>; Keir Barnbrook<sup>1</sup>; Martin Ebner<sup>1</sup>; Andrew J Creese<sup>1</sup>; <sup>1</sup>Immunocore, Abingdon, United Kingdom
- TP 623 **O-glycosylation characterization of rhTPO based on EAD mass spectrometry;** Lingsheng Chen<sup>1</sup>; Hexing Song<sup>1</sup>; Xiang Li<sup>2</sup>; Ji Luo<sup>3</sup>; Hongxu Chen<sup>1</sup>; Lihai Guo<sup>1</sup>; <sup>1</sup>SCIEX, Beijing, China; <sup>2</sup>NIFDC, Beijing, China; <sup>3</sup>SCIEX, Shanghai, China

## TUESDAY POSTERS

- samples; Evgeniy V. Petrotchenko<sup>1</sup>; Andreas Hahn<sup>2</sup>; Christoph H. Borchers<sup>1, 3, 4, 5</sup>; <sup>1</sup>Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; <sup>2</sup>Department of Pediatric Neurology, University of Giessen, Giessen, Germany; <sup>3</sup>Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; <sup>4</sup>Division of Experimental Medicine, McGill University, Montreal, QC; <sup>5</sup>Department of Pathology, McGill University, Montreal, QC
- TP 637 **In-depth O-glycosylation characterization of APOE from different expression systems — Insights for host cell selection and drug design;** Jiang Biyun<sup>1</sup>; Moyin Zhou<sup>1</sup>; Longyun Guo<sup>1</sup>; Tongdan Wang<sup>1</sup>; Jincui Huang<sup>1</sup>; <sup>1</sup>Wuxi Biologics(Shanghai) Co., Ltd., Shanghai, China
- TP 638 **Charge Variant Analysis of IgGs Directly from Cell Culture Supernatant using Microfluidic CE-ESI-MS;** J. Scott Mellors<sup>1</sup>; Adi Kulkarni<sup>2</sup>; Stephanie R. Klaubert<sup>2</sup>; Kate Yu<sup>2</sup>; Erin A. Redman<sup>1</sup>; <sup>1</sup>908 Devices Inc., Morrisville, NC; <sup>2</sup>908 Devices Inc., Boston, MA
- TP 639 **Ion mobility-mass spectrometry and collision induced unfolding methods reveal structural differences in stressed biosimilar therapeutic products;** Nicole A Rivera-Fuentes<sup>1</sup>; Matthew Vallano<sup>1</sup>; Alyssa Erlenbeck<sup>1</sup>; Michael R. Armbruster<sup>1</sup>; Amanda Cicali<sup>1</sup>; Youngseo Na<sup>2, 3</sup>; Ting Zhao<sup>2, 4</sup>; Mingeun Kim<sup>4</sup>; Anna Schwendeman<sup>4</sup>; Brandon T Ruotolo<sup>1</sup>; <sup>1</sup>University of Michigan Department of Chemistry, Ann Arbor, MI; <sup>2</sup>University of Michigan, Ann Arbor, Michigan; <sup>3</sup>Department of Medicinal Chemistry, University of Michigan, Ann Arbor, MI; <sup>4</sup>Department of Pharmaceutical Sciences, University of Michigan, Ann Arbor, MI
- TP 640 **A Data Processing Workflow Combining Orthogonal MS/MS Fragmentation Data for Comprehensive Middle-down Analysis;** Can Cui<sup>1</sup>; Aude Tartiere<sup>2</sup>; Catherine Evans<sup>3</sup>; Stephen Kok<sup>2</sup>; Yaarub Musa<sup>3</sup>; Arnd Brandenburg<sup>3</sup>; <sup>1</sup>Genedata Inc., Boston, MA; <sup>2</sup>Genedata Inc, San Francisco, CA; <sup>3</sup>Genedata AG, Basel, Switzerland
- TP 641 **Charge Variant Mass spectrometry for Analysis of biotherapeutics with Orthogonal and Fractionated sampling;** St John Skilton<sup>1</sup>; Xiaojing Shen<sup>2</sup>; Krisztina Radi<sup>1</sup>; Baburaj Kunnummal<sup>2</sup>; Kefei Wang<sup>2</sup>; <sup>1</sup>Protein Metrics, LLC, Cupertino, CA; <sup>2</sup>Bio-techno Ltd., San Jose, CA
- TP 642 **Optimized native conditions for charge variant analysis using a microfluidic CE-MS platform yield higher quality data for lower titer samples;** Hampus Engstrom<sup>1</sup>; Erin A. Redman<sup>2</sup>; J. Will Thompson<sup>2</sup>; Adi Kulkarni<sup>1</sup>; Kate Yu<sup>1</sup>; Scott Mellors<sup>2</sup>; <sup>1</sup>908 Devices Inc., Boston, MA; <sup>2</sup>908 Devices Inc., Morrisville, NC
- TP 643 **A Novel Approach to Peptide Mapping of AAV Capsid protein and Host-Cell Protein Impurities;** Sergei Saveliev<sup>1</sup>; Alba Katiria González Rivera<sup>2</sup>; Marjeta Urh<sup>2</sup>; Mike Rosenblatt<sup>2</sup>; <sup>1</sup>Promega Corporation, Madison, WI; <sup>2</sup>Promega Corporation, Madison, Wisconsin
- TP 644 **Automated Workflow Improvements for Minimizing Artificial Deamination in Peptide Mapping of Therapeutic Monoclonal Antibodies and ADCs;** Yilin Han<sup>1</sup>; Teresa Schu<sup>1</sup>; Yuanhui Ma<sup>1</sup>; Daniela Olszova<sup>1</sup>; Tawnya Flick<sup>1</sup>; Simon Letarte<sup>1</sup>; <sup>1</sup>Gilead Sciences, Oceanside, CA
- TP 645 **Utilization of Intact Reconstruction to Characterize Bi-specific antibodies;** William Resager<sup>1</sup>; Nancy Fernandes<sup>2</sup>; <sup>1</sup>Protein Metrics, Ridgefield, WA; <sup>2</sup>Lonza Biologics, Portsmouth, New Hampshire
- TP 646 **Flash Characterization of mAbs using a Combination of Reagents via Automated On-Line Microdroplet Reaction;** Michael D Knierman<sup>1</sup>; Hui Zhao<sup>2</sup>; Jim Lau<sup>2</sup>; <sup>1</sup>Agilent, Indianapolis, IN; <sup>2</sup>Agilent Technologies, Wilmington, DE
- TP 647 **Characterization of a Novel Disulfide Rich Therapeutic Antibody Fragment and determination of its SARS-Cov-2 RBD Binding Epitope by Mass Spectrometry;** Michael Bacica<sup>1</sup>; Christopher Warner<sup>2</sup>; <sup>1</sup>Primrose Bio, Inc., San Diego, CA; <sup>2</sup>Primrose Bio, Inc., San Diego, California
- TP 648 **Conformational Heterogeneity of the Monoclonal Antibody NISTmAb Investigated by Mobility-Selective CIU and Tandem-TIMS;** Fanny C Liu<sup>1</sup>; Jusung Lee<sup>1</sup>; Thais Pedrete<sup>1</sup>; Christian Bleiholder<sup>1</sup>; <sup>1</sup>Florida State University - Department of Chemistry and Biochemistry, Tallahassee, FL
- TP 649 **A middle-level approach to simplify sample preparation and data analysis for characterization of the fusion protein blinatumomab;** Lucy Fernandes<sup>1</sup>; Andreas Nägeli<sup>2</sup>; Magdalena Widgren-Sandberg<sup>2</sup>; Antony Harvey<sup>1</sup>; <sup>1</sup>ProteinMetrics LLC, Cupertino, CA; <sup>2</sup>Genovis, Kävlinge, Sweden
- TP 650 **Nano and Microscale Peptide Mapping by LC-UV-Orbitrap-Astral Detection of Monoclonal Antibodies with Fraction Collection for Detailed Analysis;** Craig P Dufresne; Thermo Fisher Scientific, West Palm Beach, FL
- PROTEINS: CONFORMATION ANALYSIS AND STRUCTURAL BIOLOGY**  
651-673
- TP 651 **Probing structural dynamic changes of dimeric nitric oxide synthase protein in response to external cues by quantitative cross-linking mass spectrometry;** Ting Jiang<sup>1</sup>; Guanghua Wan<sup>1</sup>; Haikun Zhang<sup>1</sup>; Eric Underbakke<sup>2</sup>; Changjian Feng<sup>1</sup>; <sup>1</sup>UNM College of Pharmacy, Albuquerque, NM; <sup>2</sup>Iowa State University, Ames, IA
- TP 652 **Studying the conformational interplay of different amyloid  $\beta$  peptides with native ion mobility – mass spectrometry;** Tanja Habeck<sup>1</sup>; Silvana Smilla Zurmühl<sup>1</sup>; Edvaldo Vasconcelos Soares Maciel<sup>1</sup>; Frederik Lermyte<sup>1</sup>; <sup>1</sup>Technical University of Darmstadt, Clemens-Schöpfung-Institute for Organic Chemistry and Biochemistry, Darmstadt, Germany
- TP 653 **The functional proteome landscape in aging;** Xiaojing Sui; Northwestern University, Evanston, IL
- TP 654 **Probing the formation of heterogenous photosynthetic antenna complexes from blue-green algae using native mass spectrometry;** Jaspreet K Sound<sup>1</sup>; Giorgio Bianchini<sup>2</sup>; Thrupthi Ashok<sup>1</sup>; Patricia Sánchez-Baracaldo<sup>2</sup>; Aneika C Leney<sup>1</sup>; <sup>1</sup>School of Biosciences, University of Birmingham, Birmingham, United Kingdom; <sup>2</sup>School of Geographical Sciences, University of Bristol, Bristol, United Kingdom
- TP 655 **Comprehensive analysis of SARS-CoV-2 Spike structure and function following genetic reversion reveals contribution of D614G mutation;** Lindsay E Nyhoff<sup>1</sup>; Christopher A. Haynes<sup>1</sup>; Jakub Baudys<sup>1</sup>; Theodore R. Keppel<sup>1</sup>; Sarah H. Osman<sup>1</sup>; John R. Barr<sup>1</sup>; Dongxia Wang<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA
- TP 656 **Expanding native mass spectrometry capabilities for soluble and membrane proteins using a quadrupole-ion mobility-time-of-flight mass spectrometry system;** Brad Williams<sup>1</sup>; Dale A Cooper-Shepherd<sup>2</sup>; Mario Hensen<sup>3</sup>; Jonathan T. S. Hopper<sup>3</sup>; James I. Langridge<sup>4</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>3</sup>OMass Therapeutics, Oxford, United Kingdom; <sup>4</sup>Waters Corporation, Wilmslow, United Kingdom
- TP 657 **Using In Vivo Intact Structure for System-wide Quantitative Analysis of Changes in Proteins;** Ahrum Son<sup>1</sup>; Hyunsoo Kim<sup>1, 2</sup>; Jolene K. Diedrich<sup>1</sup>; Casimir Bamberger<sup>1</sup>; Daniel B. McClatchy<sup>1</sup>; John R. Yates III<sup>1</sup>; <sup>1</sup>Scripps Research, San Diego, California; <sup>2</sup>Chungnam National University, Daejeon, South Korea
- TP 658 **Novel denaturing mass photometry approach combined to cross-linking mass spectrometry (XL-MS) to gain structural insights on a 540kDa RuvBL1/BL2-based complex;** Hugo Gizardin-Fredon<sup>1, 2</sup>; Paulo E. Santo<sup>3, 4</sup>; Marie-Eve Chagot<sup>5</sup>; Bruno Charpentier<sup>5</sup>; Tiago M. Bandejas<sup>3, 4</sup>; Xavier Manival<sup>5</sup>; Oscar Hernandez-Alba<sup>1, 2</sup>; Sarah Cianférani<sup>1, 2</sup>; <sup>1</sup>Laboratoire de Spectrométrie de Masse BioOrganique, IPHC UMR 7178, Université de Strasbourg, CNRS, Strasbourg, France; <sup>2</sup>Infrastructure Nationale de Protéomique ProFI – FR2048, Strasbourg, France; <sup>3</sup>iBET, Instituto de Biologia Experimental e Tecnológica, Oeiras, Portugal; <sup>4</sup>Instituto de Tecnologia Química e Biológica António Xavier, Universidade Nova de

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- TP 659 **Does immunopurification impair conformational and dynamical properties of proteins: the case of alpha-synuclein?**; Ines Isabel De Figueiredo; *Institut de Chimie Physique - Université Paris-Saclay, Orsay, France*
- TP 660 **Digital Quadrupole Isolation with Electron Capture Dissociation Provides Structure Information on the Transthyretin Tetramer**; Carter Lantz<sup>1</sup>; Robert Schrader<sup>1</sup>; Joseph Meeuwssen<sup>2</sup>; Rachel Franklin<sup>2</sup>; Noah Goldberg<sup>2</sup>; David Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- TP 661 **Probing Relative Flexibility of Apolipoprotein E Surface Regions by Non-specific Limited Proteolysis coupled with Mass Spectrometry**; Zachary P Del Mundo<sup>1</sup>; Vu Ngoc Huong Tran<sup>1</sup>; Haiyan Lu<sup>1</sup>; Lingjun Li<sup>1, 2</sup>; <sup>1</sup>University of Wisconsin-Madison School of Pharmacy, Madison, WI; <sup>2</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin
- TP 662 **Combining structural modeling and cross-linking mass spectrometry reveals protein binding sites within disordered regions**; Julia Ruta<sup>1</sup>; Cong Wang<sup>1</sup>; Ying Zhu<sup>1</sup>; Pin-Lian Jiang<sup>1</sup>; Boris Bogdanow<sup>1</sup>; Fan Liu<sup>1, 2</sup>; <sup>1</sup>Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; <sup>2</sup>Charité, Universitätsmedizin Berlin, Berlin, Germany
- TP 663 **Structural Proteomics Derived Structural-Activity Relationships of Novel PPARγ Inverse Agonists**; Kuang-Ting Kuo<sup>1, 2</sup>; Bilel Bdiri<sup>3</sup>; Yuanjun He<sup>3</sup>; Marcel Koenig<sup>3</sup>; Theodore Kamenecka<sup>3</sup>; Patrick R. Griffin<sup>1, 2, 3</sup>; <sup>1</sup>Department of Molecular Medicine, The Scripps Research Institute, Jupiter, FL; <sup>2</sup>Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; <sup>3</sup>Department of Molecular Medicine, The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL
- TP 664 **Effect of Ligands on Transthyretin Structure & Sub-Unit Exchange Mechanism Monitored by Native Ion Mobility Mass Spectrometry**; Robert Rider<sup>1</sup>; Carter Lantz<sup>1</sup>; Sangho Yun<sup>1</sup>; David H Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX
- TP 665 **Deep Ultraviolet Laser Protein Footprinting**; Kermit K. Murray<sup>1</sup>; Oluwatosin A. Ogundairo<sup>1</sup>; Kadeem Hayes<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA
- TP 666 **RAMP it up! Exploring conformational dynamics of the amylin 3 receptor (AMY3R) using HDX-MS**; Cameron J Fairweather<sup>1, 2</sup>; Xin Zhang<sup>1, 2</sup>; Daniel J Garama<sup>3</sup>; Patrick M Sexton<sup>1, 2</sup>; Denise Wootten<sup>1, 2</sup>; Tracy M Josephs<sup>1, 2</sup>; <sup>1</sup>Monash University, Parkville, Australia; <sup>2</sup>ARC Centre for Cryo-electron Microscopy of Membrane Proteins, Parkville, Australia; <sup>3</sup>Hudson Institute of Medical Research, Clayton, Australia
- TP 667 **Utilizing U-Shaped Mobility Analyzer (UMA) for High Performance Dust-Mite Allergen Der p2 Quality Control**; Zixin Liang<sup>1</sup>; Kang Guo<sup>2</sup>; Xiaoqiang Zhang<sup>2</sup>; Wenjian Sun<sup>2</sup>; Huilin Li<sup>1</sup>; <sup>1</sup>Sun Yat-Sen University, Guangzhou, China; <sup>2</sup>Shimadzu Research laboratory (Shanghai) Co. Ltd., Shanghai, China
- TP 668 **Covalent Modification of Cytochrome c During Thermal Unfolding and their Implications for Thermodynamic Stability Measurements**; Evelyn H MacKay-Barr<sup>1</sup>; Lars Konermann<sup>1</sup>; <sup>1</sup>University of Western Ontario, London, Ontario
- TP 669 **Mass spectrometry-based footprinting methods reveals the effect of redox partner binding on the conformational dynamics of cytochrome P450**; Mengqi Chai<sup>1</sup>; Sarah Burris-Hiday<sup>2</sup>; Emily E. Scott<sup>2</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, Saint Louis, MO; <sup>2</sup>University of Michigan, Ann Arbor, MI
- TP 670 **Transient multimers modulate conformer abundances of prion protein monomer through conformational selection: an ion mobility and mass spectrometry study**; Guillaume Van Der Rest<sup>1</sup>; Human Rezaei<sup>2</sup>; Frederic Halgand<sup>3</sup>; <sup>1</sup>Institut de Chimie Physique, Orsay, France; <sup>2</sup>INRAE, Jouy en Josas, France; <sup>3</sup>CNRS / Université Paris Saclay, Orsay, France
- TP 671 **Structural characterization of the C1 and C2 epitopes of coagulation factor VIII by X-ray Footprinting and Mass Spectrometry**; Sathi Paul<sup>1</sup>; Kenneth Childers<sup>2</sup>; Darren Kahan<sup>3</sup>; Susan Marqusee<sup>3</sup>; P. Clint Spiegel Jr<sup>2</sup>; Corie Y Ralston<sup>1</sup>; Sayan Gupta<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, CA; <sup>2</sup>Western Washington University, Bellingham, WA; <sup>3</sup>University of California, Berkeley, Berkeley, CA
- TP 672 **Development of a Web-Based Visualization tool for robust interpretation of Protein Cross-Linking**; Sanjeeva Srivastava<sup>1</sup>; Deeptarup Biswas<sup>1</sup>; Sanjyot Vinayak Shenoy<sup>1</sup>; Kamal Mandal<sup>2</sup>; Arthur Zalevsky<sup>3</sup>; Ishan Upadhyay<sup>1</sup>; Ayushi Verma<sup>1</sup>; Audrey Kishishita<sup>4</sup>; Andrej Sali<sup>4</sup>; Arun Wiita<sup>4</sup>; <sup>1</sup>IIT Bombay, Mumbai, India; <sup>2</sup>Gujarat Biotechnology University, Ahmedabad, India; <sup>3</sup>University of California San Francisco, San Francisco, CA; <sup>4</sup>University of California-San Francisco, San Francisco, CA
- TP 673 **Beamline 3.3.1 of Advanced Light Source (ALS), LBNL: A National Resource for X-ray mediated hydroxyl radical Footprinting and Mass Spectrometry**; Sayan Gupta<sup>1</sup>; Line G Kristensen<sup>1</sup>; Sathi Paul<sup>1</sup>; Brandon Russell<sup>1</sup>; Corie Y Ralston<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, CA

### PROTEOMICS: CHEMOPROTEOMICS 674-706

- TP 674 **Above-Filter Digestion Proteomics (AFDIP) identifies drug targets and estimates ligand binding site**; Bohdana Sokolova<sup>1</sup>; Amir Ata Saei<sup>1</sup>; Hassan Gharibi<sup>1</sup>; Maryam Jafari<sup>1</sup>; Hezheng Lyu<sup>1</sup>; Massimiliano Gaetani<sup>1</sup>; Roman Zubarev<sup>1</sup>; <sup>1</sup>Karolinska Institutet, Stockholm, Sweden
- TP 675 **Protein a-N-methylation promotes nucleocytoplasmic transport of aminoacyl-tRNA**; Qianqing Zhang<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>UC Riverside, Riverside, CA
- TP 676 **Automated High-throughput Activity-based Protein Profiling Facilitates Covalent Drug Discovery**; Yumeng Li<sup>1</sup>; Zhenze Jiang<sup>1</sup>; <sup>1</sup>Roche, Shanghai, China
- TP 677 **Enabling activity-based protein profiling (ABPP) for drugs that form disulfides: identification of off-targets for ALS and alcohol abuse drugs**; Durgalakshmi Sivasankar<sup>1</sup>; Wensheng Yang<sup>1</sup>; Jeffrey Agar<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA
- TP 678 **High-throughput profiling of compound-induced proteome thermal stability changes**; Alexey Chernobrovkin<sup>1</sup>; Daniel Martinez Molina<sup>1</sup>; <sup>1</sup>Pelago Bioscience AB, Solna, Sweden
- TP 679 **Getting the Most Out of Thermal Proteome Profiling: Comparison of R Packages for Data Analysis**; Connor P Jewell<sup>1</sup>; Massimiliano Bissa<sup>2</sup>; Andrew J Perciaccante<sup>1</sup>; Genoveffa Franchini<sup>2</sup>; Daniel H Appella<sup>3</sup>; Lisa M Jenkins<sup>1</sup>; <sup>1</sup>Laboratory of Cell Biology, Center for Cancer Research, National Cancer Institute, Bethesda, MD; <sup>2</sup>Vaccine Branch, Center for Cancer Research, National Cancer Institute, Bethesda, MD; <sup>3</sup>Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD
- TP 680 **Chemical Proteomic Strategy Utilizing a Photoreactive Chloroalkane Capture Tag for Target Discovery**; Alba Katiria González Rivera<sup>1</sup>; Robin Hurst<sup>1</sup>; Sergiy Levin<sup>2</sup>; Michael M. Rosenblatt<sup>1</sup>; Rachel Friedman Ohana<sup>1</sup>; <sup>1</sup>Promega Corporation, Madison, WI; <sup>2</sup>Firmenich SA, R&D North America, San Diego, California
- TP 681 **Unbiased identification of SAMT-247 reaction sites on proteins in cell lysates**; Tapan K. Maity<sup>1</sup>; Connor P. Jewell<sup>1</sup>; Andrew J. Perciaccante<sup>1</sup>; Daniel H. Appella<sup>2</sup>; Lisa M. Jenkins<sup>1</sup>; <sup>1</sup>Laboratory of Cell Biology, Center for Cancer Research, National Cancer Institute, Bethesda, MD; <sup>2</sup>National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD

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- TP 682 **Rescue of  $\Delta F508$ -CFTR trafficking in cystic fibrosis through a QPCT-dependent pathway;** Le Sun; *the Scripps Research Institute, San Diego, CA*
- TP 683 **Misfolded Protein Profiling Reveals the Protein Targets of Cellular Manganese and Vanadium Exposure;** Guy M. Quanrud<sup>1</sup>; Macon Abernathy<sup>1</sup>; Samantha C. Ying<sup>1</sup>; Joseph Genereux<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- TP 684 **Confluence of Safeguards: A Chemoproteomic Platform for Highly Sensitive and Selective Citrulline Mapping in Alzheimer's Disease;** Wei Wilson Li<sup>1</sup>; Zexin Zhu<sup>1</sup>; Haiyan Lu<sup>1</sup>; Zicong Wang<sup>1</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>University of Wisconsin-Madison School of Pharmacy, Madison, WI; <sup>2</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin
- TP 685 **Uniting global and subcellular-localized redox proteomics to uncover redox-sensitive cysteine regulators of stress granule dynamics;** Ashley Julio<sup>1</sup>; Katarina Cohen<sup>1</sup>; Keriann M Backus<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles
- TP 686 **Cysteine-reactive electrophilic compounds remodel the proteome by modulating cellular proteostasis processes;** Flowreen Shikwana<sup>1</sup>; Ashley Julio<sup>1</sup>; Cindy Truong<sup>1</sup>; Nikolas Burton<sup>1</sup>; Emil R. Dominguez<sup>1</sup>; Alexandra C. Turmon<sup>1</sup>; Jian Cao<sup>1</sup>; Keriann M Backus<sup>1</sup>; <sup>1</sup>University of California, Los Angeles, Los Angeles, CA
- TP 687 **CIAA: Integrated Proteomics and Structural Modeling for Predicting Cysteine Reactivity with Iodoacetamide Alkyne;** Lisa M Boatner<sup>1</sup>; Jerome Eberhardt<sup>2</sup>; Jose O Castellon<sup>1</sup>; Flowreen Shikwana<sup>1</sup>; Kendall N Houk<sup>1</sup>; Stefano Forli<sup>2</sup>; Keriann M Backus<sup>1</sup>; <sup>1</sup>University of California Los Angeles, Los Angeles, CA; <sup>2</sup>Scripps Research Institute, San Diego
- TP 688 **Increasing the Throughput and Depth of Cell-Based Cysteine Ligandability Profiling Studies with Automation and Intelligent Data Acquisition;** Hanna Budayeva; *Genentech Inc., South San Francisco*
- TP 689 **Mass Spectrometry-Aided Identification and Characterization of Helicase Binders That Can Irreversibly Bind to a Transient Pocket and Inhibit Activity;** Jeremiah J Bowers<sup>1</sup>; Doug McLaughlin<sup>2</sup>; Dave M. Garby<sup>1</sup>; Brian Sosa<sup>2</sup>; William LaMarr<sup>1</sup>; Peter Rye<sup>1</sup>; Bini Ramachandran<sup>1</sup>; <sup>1</sup>Momentum Biotechnologies, Billerica, MA; <sup>2</sup>MOMA Therapeutics, Cambridge, MA
- TP 690 **Application of chemoproteomics for the preclinical characterization of highly selective and potent covalent BTK inhibitors;** Bekim Bajrami; *Biogen, Cambridge, MA*
- TP 691 **Unbiased compound selectivity profiling using high throughput CETSA MS;** Alexey Chernobrovkin<sup>1</sup>; Tuomas A Tolvanen<sup>1</sup>; Tomas Friman<sup>1</sup>; Christina Velasco<sup>1</sup>; Daniel Martinez Molina<sup>1</sup>; <sup>1</sup>Pelago Bioscience AB, Solna, Sweden
- TP 692 **An Automated Proteome Integral Solubility Alteration (PISA) Workflow Using DIA for Increased Throughput and Robustness;** Keith D Rivera<sup>1</sup>; Isabelle A Kressy<sup>1</sup>; Natalie M Clark<sup>1</sup>; D. R. Mani<sup>1</sup>; Namrata D. Udeshi<sup>1</sup>; Steven A Carr<sup>1</sup>; <sup>1</sup>Broad Institute, Cambridge, MA
- TP 693 **Bromo-desthiobiotin tag (Br-DTB) for unbiased profiling of chemical modification sites in human proteome;** Bibhuti Bhusana Palai<sup>1</sup>; Zongtao Lin<sup>1</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>Washington University School of Medicine, St. Louis, MO
- TP 694 **Comparing serum protein profiles of Homo sapiens with Pan troglodytes via Label-free MS proteomics: How similar are we?;** Marcos N Eberlin<sup>1</sup>; Mariana Sá<sup>2</sup>; Iasmim Lopes Lima<sup>1</sup>; Thais Regiane Cataldi<sup>3</sup>; Esther Olabisi-Adeniyi<sup>2</sup>; Jennifer Geddes-McAlister<sup>2</sup>; <sup>1</sup>Mackenzie University, São Paulo, Brazil; <sup>2</sup>University of Guelph, GUELPH, ON; <sup>3</sup>Universidade de São Paulo, Piracicaba, Brazil
- TP 695 **Proteomics and bioinformatics reveal anandamide antinociceptive effects are mediated by vanilloid receptors in Caenorhabditis elegans;** Marzieh Abdollahi<sup>1</sup>; Jennifer Ben Salem<sup>1</sup>; Jesus D Castano<sup>1</sup>; Francis Beaudry<sup>1</sup>; <sup>1</sup>Universite de Montreal, St-Hyacinthe, QC
- TP 696 **Exploring sample preparation workflows and instrument acquisitions for chemoproteomic global protein profiling;** Taylor P. Ma<sup>1</sup>; Meena Choi<sup>1</sup>; Felipe Da Veiga Leprevost<sup>1</sup>; Nicolas Hartel<sup>2</sup>; Jana Richter<sup>2</sup>; Hanna G. Budayeva<sup>1</sup>; <sup>1</sup>Genentech, Inc., South San Francisco, CA; <sup>2</sup>ThermoFisher Scientific, San Jose, CA
- TP 697 **Polymerase  $\kappa$  Recruits DDX23 to Promote R-loop Resolution;** Feng Tang<sup>1</sup>; Yinan Wang<sup>2</sup>; Yinsheng Wang<sup>2</sup>; <sup>1</sup>University of California, riverside, Riverside, CA; <sup>2</sup>UC Riverside, Riverside, CA
- TP 698 **An ultra-deep, cysteine-profiling approach for chemoproteomics powered by TMT and the new Astral mass analyzer;** Ka Yang<sup>1</sup>; Qing Yu<sup>1</sup>; Shane L. Dawso<sup>1</sup>; Rebecca L. Whitehouse<sup>1</sup>; Lu Zhang<sup>2</sup>; Jeffrey G. Martin<sup>2</sup>; Douglas S. Johnson<sup>2</sup>; Joao A. Paulo<sup>1</sup>; Steven Gygi<sup>1</sup>; <sup>1</sup>Harvard Medical School, Boston, MA; <sup>2</sup>Biogen, Cambridge, MA
- TP 699 **Leveraging Data Independent Acquisition (DIA) for Cysteine Targeting and Proteome Profiling;** Lara Holoidovsky<sup>1</sup>; Tianyang Yan<sup>1</sup>; Weixian Deng<sup>1</sup>; James Wohlschlegel<sup>1</sup>; Keriann M Backus<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles
- TP 700 **Fast Photochemical Iodination and Capture by Suzuki as a Novel Tyrosine Chemoproteomics Method;** Miranda Villanueva<sup>1</sup>; Nikolas Burton<sup>1</sup>; Andrew Becker<sup>1</sup>; Eli Bilech<sup>1</sup>; Sho Takechi<sup>1</sup>; Keriann M Backus<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles, CA
- TP 701 **Generating Cysteine-Trypsin Cleavage Sites With 2-Chloroacetamide Capping;** Samuel Ofori<sup>1</sup>; Heta Desai<sup>2</sup>; Flowreen Shikwana<sup>1</sup>; Lisa Boatner<sup>1</sup>; Jose O Castellon<sup>1</sup>; Keriann M Backus<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles, California; <sup>2</sup>Gristone Bio, Boston, USA, Massachusetts
- TP 702 **Probing the Target Site for a Promising Acaricide to Tackle Varroa Mites in Honeybee Colonies;** Osei Boakye Fordwour<sup>1</sup>; Niloufar Choudbdar<sup>2</sup>; Laura Gleeson<sup>2</sup>; Erika Plettner<sup>2</sup>; Leonard J Foster<sup>1</sup>; <sup>1</sup>UBC, Vancouver, BC; <sup>2</sup>Simon Fraser University, Burnaby, BC
- TP 703 **From seeding to separation: a 96-well format sample preparation protocol for cell-based high throughput proteomics;** Julia E Robbins<sup>1</sup>; Andrea I Gutierrez<sup>2</sup>; J. Sebastian Paez<sup>2</sup>; Daniele Canzani<sup>2</sup>; Bodhi Hueffmeier<sup>2</sup>; Brian McEllin<sup>2</sup>; Carolyn Allen<sup>2</sup>; Yang Gao<sup>2</sup>; Tonibelle Gatbonton-Schwager<sup>2</sup>; William E Fondrie<sup>2</sup>; Alexander J Federation<sup>2</sup>; Lindsay K Pino<sup>2</sup>; <sup>1</sup>Talus Bioscience, Seattle; <sup>2</sup>Talus Bioscience, Seattle, WA
- TP 704 **A Chemoproteomic Approach to Identifying Biologically Active Cyclic Peptides;** Katrina H. Andrews<sup>1</sup>; Haley Gauer<sup>1</sup>; Nikolas R. Burton<sup>1</sup>; Keriann M. Backus<sup>1</sup>; <sup>1</sup>University of California, Los Angeles, Los Angeles, CA
- TP 705 **Developing a minimalist proximity labeling method using the short tetracysteine tag;** Elijah B. Bilech<sup>1,2</sup>; Andrew P. Becker<sup>1,2</sup>; Tomoyuki Fukuta<sup>3,4</sup>; Keriann M. Backus<sup>1,2</sup>; <sup>1</sup>Department of Biological Chemistry, David Geffen School of Medicine, UCLA, Los Angeles, CA; <sup>2</sup>Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA; <sup>3</sup>Department of Chemistry, School of Science, The University of Tokyo, Tokyo, Japan; <sup>4</sup>Graduate School of Pharmaceutical Sciences, The University of Tokyo, Tokyo, Japan
- TP 706 **Advancing the discovery of novel senolytics through cysteine-focused activity-based protein profiling;** Matthew White<sup>1,2</sup>; Jesús Gil<sup>2,3</sup>; Edward W. Tate<sup>4,5</sup>; <sup>1</sup>Imperial College London, London, United Kingdom; <sup>2</sup>MRC London Institute of Medical Sciences (LMS), London, United Kingdom; <sup>3</sup>Institute of Clinical Sciences (ICS), Faculty of Medicine, Imperial College London, London, United Kingdom; <sup>4</sup>Imperial College London, London, United Kingdom; <sup>5</sup>Francis crick institute, London, United Kingdom

### PROTEOMICS: CLINICAL APPLICATIONS I 707-729

- TP 707 **Proteomic evidence that Heimdall, an alternative protein from a non-coding RNA knockout, switches astrocytes to a neural stem cell phenotype;** Alice Capuz<sup>1,2</sup>; Isabelle Fournier<sup>1</sup>; Franck Rodet<sup>1</sup>; Michel Salzet<sup>1</sup>; <sup>1</sup>Laboratoire



## TUESDAY POSTERS

- PRISM, Inserm U1192, Université de Lille, Villeneuve d'Ascq Cedex, France; <sup>2</sup>Brigham and Women's Hospital, Boston, MA*
- TP 708 **Data-independent acquisition mass spectrometry analysis of serum proteomic profiles in chronic obstructive pulmonary disease;** Wen-Yi Liu<sup>1</sup>; Sheng-Ming Wu<sup>1</sup>; Kuan-Yuan Chen<sup>1</sup>; Kang-Yun Lee<sup>1</sup>; Chia-Li Han<sup>1</sup>; <sup>1</sup>Taipei Medical University, Taipei, Taiwan
- TP 709 **Ultra-deep Monitoring of Human and Pig Proteins in Blood Serum Yields Novel Insights into the Dynamics of Pig Kidney Xenotransplantation;** Alexey Stukalov<sup>1</sup>; Brittany Lee<sup>1</sup>; Khatereh Motamedchaboki<sup>2</sup>; Brian D. Piening<sup>3</sup>; Eloi Schmauch<sup>4</sup>; Simon Williams<sup>5, 6</sup>; Ian Jaffe<sup>3, 5</sup>; Maedeh Mohebnasab<sup>7</sup>; Alexa Dowdell<sup>3</sup>; Adam Griesemer<sup>5, 6</sup>; Karen Khalil<sup>5, 6</sup>; Jacqueline I. Kim<sup>3, 5</sup>; David Ayares<sup>8</sup>; Marc Lorber<sup>9</sup>; Massimo Mangiola<sup>5, 10</sup>; Vasishta Tatapudi<sup>5, 11</sup>; Jeffrey M. Stern<sup>5, 6</sup>; Jef D. Boeke<sup>12</sup>; Harvey I. Pass<sup>6</sup>; Robert A. Montgomery<sup>5, 6</sup>; Serafim Batzoglou<sup>1</sup>; Asim Siddiqui<sup>1</sup>; Brendan J. Keating<sup>5, 6</sup>; <sup>1</sup>Seer Inc., Redwood City, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Earle A. Childs Research Institute, Providence Cancer Institute, Portland, OR; <sup>4</sup>Broad Institute of MIT and Harvard, Boston, MA; <sup>5</sup>NYU Langone Transplant Institute, NYU Langone Health, New York, NY; <sup>6</sup>Department of Surgery, NYU Grossman School of Medicine, New York, NY; <sup>7</sup>Division of Molecular & Genomic Pathology, University of Pittsburgh Medical Center, Pittsburgh, PA; <sup>8</sup>Revivicor Inc., Blacksburg, VA; <sup>9</sup>United Therapeutics, Silver Spring, MD; <sup>10</sup>Department of Pathology, NYU Grossman School of Medicine, New York, NY; <sup>11</sup>Department of Medicine, NYU Grossman School of Medicine, New York, NY; <sup>12</sup>Institute for Systems Genetics, NYU Langone Health, New York, NY
- TP 710 **Large-scale pan-cancer study elucidates the proteomic profile of 1261 FFPE tumour samples;** Stephan Eckert<sup>1, 2</sup>; Johanna Tueshaus<sup>1</sup>; Marius Schliemann<sup>1</sup>; Matthew The<sup>1</sup>; Peer-Hendrik Kuhn<sup>3</sup>; Carolin Mogler<sup>3</sup>; Bernhard Kuster<sup>1, 2, 4</sup>; <sup>1</sup>Technical University of Munich (TUM), Freising, Germany; <sup>2</sup>DKFZ German Cancer Research Center, Heidelberg, Germany; <sup>3</sup>Technical University of Munich (TUM), Munich, Germany; <sup>4</sup>Bavarian Center for Biomolecular Mass Spectrometry (BayBioMS), Freising, Germany
- TP 711 **Differentiating AL amyloidosis from immunoglobulin light chain deposition disease utilizing histopathology and mass spectrometry-based proteomics;** A Cooper Walland<sup>1</sup>; Anna Liu<sup>1</sup>; Mirian Barbosa<sup>1</sup>; Ahmet Dogan<sup>1</sup>; Jessica Chapman<sup>1</sup>; <sup>1</sup>Memorial Sloan Kettering Cancer Center, New York, NY
- TP 712 **Biomarker Discovery and Quantitation Guided by a Data Independent Acquisition (DIA) Mass Spectrometry Technique;** Ling Li<sup>1</sup>; Sumit Bhutada<sup>2</sup>; Nicolas Piuzzi<sup>3</sup>; Belinda Willard<sup>1</sup>; Suneel Apte<sup>2</sup>; <sup>1</sup>Department of Shared Laboratory Resources, Cleveland Clinic, Cleveland, Ohio; <sup>2</sup>Department of Biomedical Engineering, Cleveland Clinic, Cleveland, Ohio; <sup>3</sup>Department of Orthopaedic Surgery, Cleveland, Ohio
- TP 713 **Standardized, fully automated undepleted plasma and MagNet enrichment workflows enabled by the Evotip Pure;** Joel Vej-Nielsen<sup>1</sup>; Magnus Huusfeldt<sup>1</sup>; Stoyan Stoychev<sup>1</sup>; Dorte B. Bekker-Jensen<sup>1</sup>; Nicolai Bache<sup>1</sup>; <sup>1</sup>EvoSep, Odense, Denmark
- TP 714 **IonStar-based Clinical Proteomics Pipeline Enables Identification of Novel Biomarkers for Bacterial Exacerbation of Chronic Obstructive Pulmonary Disease;** Xiaoyu Zhu<sup>1</sup>; Shuo Qian<sup>2</sup>; Shichen Shen<sup>1</sup>; Sanjay Sethi<sup>1</sup>; Gordon Broderick<sup>3</sup>; Jun Qu<sup>1, 4</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY; <sup>2</sup>Roswell Park Comprehensive Cancer Center, Buffalo, NY; <sup>3</sup>Rochester General Hospital, Rochester, New York; <sup>4</sup>New York State Center of Excellence in Bioinformatics and Life Sciences, Buffalo, New York
- TP 715 **Optimizing LC-MS/MS settings for plasma proteomics analysis with cap-flow LC separation and dia-PASEF;** Andreas Schmidt<sup>1</sup>; Claudia Martelli<sup>2</sup>; Raphael Schuster<sup>1</sup>; Schmit Pierre-Olivier<sup>3</sup>; Markus Lubeck<sup>1</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; <sup>2</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>3</sup>Bruker Daltonique S.A., Wissembourg, France
- TP 716 **Quantification of Her2 expression in Her2-low tumors by targeted mass spectrometry;** Negarsadat Mostolizadeh<sup>1</sup>; Neginsadat Mostolizadeh<sup>1</sup>; Gerald Batist<sup>2, 3, 4</sup>; Mark Basik<sup>2, 3, 4, 5</sup>; Christoph H. Borchers<sup>1, 2, 3, 6</sup>; <sup>1</sup>Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; <sup>2</sup>Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; <sup>3</sup>Division of Experimental Medicine, McGill University, Montreal, QC; <sup>4</sup>Department of Oncology, McGill University, Montreal, QC; <sup>5</sup>Department of Surgery, McGill University, Montreal, QC; <sup>6</sup>Department of Pathology, McGill University, Montreal, QC
- TP 717 **No automation? No problem! An optimized, simplified workflow for the targeted proteomic analysis of fibrinogen in 4,200 plasma samples;** Carly A. L. Twigg<sup>1</sup>; Joohyun Ryu<sup>1</sup>; Stefani N. Thomas<sup>1</sup>; <sup>1</sup>Department of Laboratory Medicine and Pathology, University of Minnesota School of Medicine, Minneapolis, MN
- TP 718 **Novel scavengers unbiasedly quadruple FFPE protein yields for clinical proteogenomics;** Matthew Holt<sup>1</sup>; Craig T. Vollert<sup>1</sup>; George Miles<sup>1, 2</sup>; Eric C. Chang<sup>1, 3</sup>; Charles E Foulds<sup>1, 4</sup>; Bing Zhang<sup>1, 2</sup>; <sup>1</sup>Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; <sup>2</sup>Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, Texas; <sup>3</sup>Department of Molecular and Cellular Biology, Baylor College of Medicine, Houston, Texas; <sup>4</sup>Department of Medicine, Baylor College of Medicine, Houston, Texas
- TP 719 **Optimizing Capivasertib Response Prediction in Cancer: Unveiling Resistance Mechanisms through Precision Proteomics;** Neginsadat Mostolizadeh<sup>1</sup>; Negarsadat Mostolizadeh<sup>1</sup>; Gerald Batist<sup>2, 3, 4</sup>; Mark Basik<sup>3, 4, 5, 6</sup>; Christoph H. Borchers<sup>1, 2, 3, 7</sup>; <sup>1</sup>Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; <sup>2</sup>Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; <sup>3</sup>Division of Experimental Medicine, McGill University, Montreal, QC; <sup>4</sup>Department of Oncology, McGill University, Montreal, QC; <sup>5</sup>Gerald Bronfman Department of Oncology, McGill University, Montreal, QC; <sup>6</sup>Department of Surgery, McGill University, Montreal, QC; <sup>7</sup>Department of Pathology, McGill University, Montreal, QC
- TP 720 **Identification of 15-keto-PGE2 post-translational protein modifications by LC/MS/MS to study an anti-inflammatory therapy;** Fu-An Li<sup>1</sup>; Ling-Hui Wang<sup>1</sup>; <sup>1</sup>Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan
- TP 721 **Efficient analysis of phosphopeptides from lung cancer tissues on a silica-based monolithic column and timsTOF;** Bella Bruszel<sup>1</sup>; Fanni Bugyi<sup>2</sup>; Goran Mitulovic<sup>3</sup>; Michael Krawitzky<sup>3</sup>; Gary Kruppa<sup>4</sup>; Arnel Nicolas<sup>1</sup>; Lilla Turiak<sup>2</sup>; <sup>1</sup>Institute of Science and Technology, Maria Gugging, Austria; <sup>2</sup>HUN-REN Research Centre for Natural Sciences, Budapest, Hungary; <sup>3</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>4</sup>Bruker S.R.O., Brno, Czech Republic
- TP 722 **Turbocharging Discovery: Crafting a High-Speed, High-Efficiency Monolithic Column for Breakneck Single-Cell Analysis;** Ruben Shrestha<sup>1</sup>; Michael Krawitzky<sup>2, 3</sup>; Simion Kreimer<sup>4</sup>; Goran Mitulovic<sup>3</sup>; Ali Haghani<sup>4</sup>; Jennifer E. Van Eyk<sup>4</sup>; Gary Kruppa<sup>5</sup>; <sup>1</sup>Bruker Scientific LLC, San Jose, CA; <sup>2</sup>Bruker Daltonics, San Jose, CA; <sup>3</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>4</sup>Cedars-Sinai Medical Center, Los Angeles; <sup>5</sup>Bruker S.R.O., Brno, Czech Republic
- TP 723 **Development and application of quantitative proteomics for assessing preclinical and clinical pharmacodynamic activity of a potent STAT3 protein degrader;** Eric Kuhn<sup>1</sup>; Sarah Martinez<sup>1</sup>; Joyoti Dey<sup>1</sup>; Alyssa Fasciano<sup>1</sup>; Christine Klaus<sup>1</sup>; Susanne Breitkopf<sup>1</sup>; Yatao Shi<sup>1</sup>; Dirk Walther<sup>1</sup>; Yi-Ting Wang<sup>1</sup>; Chris Browne<sup>1</sup>; Dapeng Chen<sup>1</sup>; Beccy Mosher<sup>1</sup>;

## TUESDAY POSTERS

- Jared Gollob<sup>1</sup>; Juliet Williams<sup>1</sup>; Kirti Sharma<sup>1</sup>; <sup>1</sup>*Kymera Therapeutics, Watertown, MA*
- TP 724 **A multimodal approach determining effects of estrogen receptor alpha (ER $\alpha$ ) inhibition in mouse models of benign prostatic hyperplasia;** Hannah Miles<sup>1, 2, 3</sup>; Elliot Patrenets<sup>3, 4</sup>; William A. Ricke<sup>1, 2, 3, 5</sup>; Lingjun Li<sup>6, 7</sup>; <sup>1</sup>*School of Pharmacy, University of Wisconsin-Madison, Madison, WI*; <sup>2</sup>*Department of Urology, UW-Madison, Madison, WI*; <sup>3</sup>*George M. O'Brien Urology Research Center, UW-Madison, Madison, WI*; <sup>4</sup>*Department of Integrative Biology, UW-Madison, Madison, WI*; <sup>5</sup>*School of Medicine and Public Health, UW-Madison, Madison, WI*; <sup>6</sup>*School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin*; <sup>7</sup>*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*
- TP 725 **Advancement in nanoparticle-based proteomic analysis of whole blood obtained from various dried blood spot collection devices;** Maedeh Zamani<sup>1</sup>; Brittany Lee<sup>1</sup>; Shao-Yung Chen<sup>1</sup>; Shadi Ferdosi<sup>1</sup>; Xiaoyuan Zhou<sup>1</sup>; Daniel Hornburg<sup>1</sup>; Aaron Steven Gajadhar<sup>1</sup>; <sup>1</sup>*Seer Inc., Redwood City, CA*
- TP 726 **LC-SRM and machine learning allowing fast detection of urinary tract infections;** Clarisse Gotti<sup>1</sup>; Florence Roux-Dalvai<sup>1</sup>; Antoine Lacombe-Rastoll<sup>1</sup>; Cristina Jacob<sup>2</sup>; Eve Bérubé<sup>3</sup>; Maurice Boissinot<sup>3</sup>; Michel G. Bergeron<sup>3</sup>; Neloni Wijeratne<sup>2</sup>; Claudia Martins<sup>2</sup>; Arnaud Droit<sup>1</sup>; <sup>1</sup>*Proteomics Platform and Computational Biology laboratory, CHU de Québec Université Laval Research Center, Québec, QC*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*Infectiology Research Centre, CHU de Québec Université Laval Research Center, Québec, QC*
- TP 727 **In-depth proteomic analysis of mouse inner ear for the studies of age-related hearing loss;** Samon Nagatani<sup>1</sup>; Maiko Okamura<sup>1</sup>; Yoko Fukunaga<sup>2</sup>; Shuji Yamashita<sup>1</sup>; Takashi Nirasawa<sup>3</sup>; Hiroki Kato<sup>4</sup>; Kengo Yoshii<sup>4</sup>; Norio Yamamoto<sup>2, 5</sup>; Masaya Ikegawa<sup>1</sup>; <sup>1</sup>*Doshisha University, Kyotanabe, Japan*; <sup>2</sup>*Kyoto university, Sakyo-ku, Japan*; <sup>3</sup>*Bruker Japan K.K., Yokohama, Japan*; <sup>4</sup>*Kyoto Prefectural University of Medicine, Kamigyo-ku, Japan*; <sup>5</sup>*Kobe City Medical Center General Hospital, Kobe, Japan*
- TP 728 **Utility of novel capillary-based blood collection devices as alternatives to venipuncture for a new MRM clinical proteomic assay;** Sarah Phillips<sup>1</sup>; Abby Richard<sup>1</sup>; Alicia Patrick<sup>1</sup>; Cara Kifer<sup>1</sup>; Danielle Dvorak<sup>1</sup>; Merrie Ann O'Brien<sup>1</sup>; Sierra Whitted<sup>1</sup>; Gary Pestano<sup>2</sup>; Laura Peek<sup>1</sup>; <sup>1</sup>*Biodesix, De Soto, KS*; <sup>2</sup>*Biodesix, Louisville, CO*
- TP 729 **Utility of a Novel Blood Storage Device for Clinical Proteomics and its Effect on the Plasma Proteome;** Colin T McDowell<sup>1</sup>; Amanda Weaver<sup>1</sup>; Gary Pestano<sup>1</sup>; <sup>1</sup>*Biodesix, Louisville, CO*
- PROTEOMICS: INFECTIOUS DISEASES**  
730-734
- TP 730 **Multi-omics reveals that Sirt2 and Sirt5 differentially control macrophage polarization;** Hui Tang<sup>1</sup>; Tuvshintugs Baljinnyam<sup>1</sup>; Abhishek Mishra<sup>2</sup>; Chinnaswamy Jagannath<sup>2</sup>; Kangling Zhang<sup>1</sup>; <sup>1</sup>*University of Texas Medical Branch at Galveston, Galveston, TX*; <sup>2</sup>*Houston Methodist Research Institute & Weill Cornell Medical College, Houston, Texas*
- TP 731 **Kinetic analysis and ultrasensitive detection of SARS-CoV-2 3CLpro-mediated proteolysis.;** Peter A Bell<sup>1</sup>; Kevin Yang<sup>2</sup>; Reinhild Kappelhoff<sup>1</sup>; Julia Kraegenbring<sup>3</sup>; Amirmansoor Hakimi<sup>2</sup>; Hugo Cesar Ramos De Jesus<sup>1</sup>; Brett Larsen<sup>4</sup>; Rosa Viner<sup>2</sup>; Christopher M Overall<sup>1</sup>; <sup>1</sup>*University of British Columbia, Vancouver, BC*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*Thermo Fisher Scientific GmbH, Bremen, Germany*; <sup>4</sup>*Thermo Fisher Scientific, Toronto, ON*
- TP 732 **Polymycovirus Alteration of Virulence Factors in Aspergillus fumigatus: A Mass Spectrometric Proteomics Study ;** Catalina Avendaño<sup>1</sup>; Sydney Nguyen<sup>1</sup>; Ioly Kotta-Loizou<sup>2, 3</sup>; Gabriele Sass<sup>4</sup>; Daniel Röth<sup>1</sup>; David A. Stevens<sup>4, 5</sup>; Markus Kalkum<sup>1</sup>; <sup>1</sup>*City of Hope, Beckman Research Institute. Department of Immunology and*
- Theranostics, Duarte, CA*; <sup>2</sup>*Imperial College London, Faculty of Natural Sciences, Department of Life Sciences & University of Hertfordshire, School of Life and Medical Sciences, Department of Clinical, Pharmaceutical and Biological Science, London, United Kingdom*; <sup>3</sup>*University of Hertfordshire, School of Life and Medical Sciences, Department of Clinical, Pharmaceutical and Biological Science, London, United Kingdom*; <sup>4</sup>*California Institute for Medical Research, San Jose, CA*; <sup>5</sup>*Stanford University School of Medicine, Division of Infectious Diseases and Geographic Medicine, Stanford, CA*
- TP 733 **Targeting G9a Regulated m6A RNA Modification Pathway to Hinder SARS-CoV-2 Replication;** Adil Muneer<sup>1</sup>; Ling Xie<sup>2</sup>; Feng Zhang<sup>3</sup>; Xuping Xie<sup>4</sup>; John A Wrobel<sup>2</sup>; Yan Xiong<sup>5</sup>; Xufen Yu<sup>5</sup>; Charles Wang<sup>6</sup>; Ciprian Gheorghie<sup>6</sup>; Ping Wu<sup>4</sup>; Hongjun Song<sup>3</sup>; Jin Jian<sup>5</sup>; Pei-Yong Shi<sup>4</sup>; Xian Chen<sup>2</sup>; <sup>1</sup>*University of North Carolina Chapel Hill, Chapel Hill, NC*; <sup>2</sup>*University of North Carolina at Chapel Hill, Chapel Hill, NC*; <sup>3</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>4</sup>*University of Texas Medical Branch at Galveston, Galveston, TX*; <sup>5</sup>*Icahn School of Medicine at Mount Sinai, New York, NY*; <sup>6</sup>*Loma Linda University, Loma Linda, CA*
- TP 734 **Vitamin B12 physiology and metalloproteome changes in the pathogen Pseudomonas aeruginosa across environmental gradients;** Viktoria Steck<sup>1</sup>; Matthew R. McIlvin<sup>1</sup>; Mak A Saito<sup>1</sup>; <sup>1</sup>*Woods Hole Oceanographic Institution, Falmouth, MA*
- PROTEOMICS: NEW APPROACHES II**  
735-754
- TP 735 **A new strategy for screening disease-associated proteins by MS based on drug and protein interactions;** Weibing Zhang<sup>1</sup>; Yini Pan<sup>1</sup>; Zhenxin Wang<sup>2</sup>; Zhichao Yan<sup>1</sup>; Haofan Sun<sup>3</sup>; Lingyi Zhang<sup>1</sup>; <sup>1</sup>*East China University of Science and Technology, Shanghai, China*; <sup>2</sup>*Zhongshan Hospital Fudan University, Shanghai, China*; <sup>3</sup>*Beijing Proteome Research Center, Beijing, China*
- TP 736 **Real-time Isotopic Signature Targeted Profiling;** Guogeng Jia<sup>1</sup>; Yicheng Liu<sup>1</sup>; Tianyu Feng<sup>1</sup>; Chu Wang<sup>1</sup>; <sup>1</sup>*Peking University, Beijing, China*
- TP 737 **Pursuing Options In Parallel: Multiplexed In Vivo Screening Using Peptide Tagging with mRNA;** Jason Thall<sup>1</sup>; Lisa Crawford<sup>1</sup>; Jonathan Hoggatt<sup>1</sup>; <sup>1</sup>*Moderna, Cambridge, MA*
- TP 738 **Bottom-Up Proteomics of Human Keratinocytes Exposed to 4,4'-Methylene Diphenyl Diisocyanate-Glutathione Conjugates by Off-Line MuDPIT;** Brandon F Law<sup>1</sup>; Chen-Chung Lin<sup>1</sup>; Justin M. Hettick<sup>1</sup>; <sup>1</sup>*Centers for Disease Control, NIOSH, Morgantown, WV*
- TP 739 **Improving complex phosphopeptide characterization with hybrid electron activated dissociation and collision-induced dissociation fragmentation;** Patrick Pribil<sup>1</sup>; Loren Olsen<sup>2</sup>; Jeremy Potriquet<sup>3</sup>; Daniel Winter<sup>4</sup>; <sup>1</sup>*SCIEX, Concord, ON*; <sup>2</sup>*SCIEX, Redwood City, CA*; <sup>3</sup>*SCIEX, Mulgrave, Australia*; <sup>4</sup>*All G Foods, Waterloo, Australia*
- TP 740 **An Automated Sample Preparation Workflow for Proteomic Profiling of Membrane-Bound Vesicles from Urine;** Ireshyn Govender<sup>1</sup>; Sindisiwe Buthelezi<sup>2</sup>; Previn Naicker<sup>2</sup>; Andrea Ellero<sup>1, 3</sup>; Justin Jordaan<sup>1</sup>; Stoyan Stoychev<sup>1, 4</sup>; <sup>1</sup>*ReSyn Biosciences, Pretoria, South Africa*; <sup>2</sup>*Council for Scientific and Industrial research, Pretoria, South Africa*; <sup>3</sup>*University of Pretoria, Pretoria, South Africa*; <sup>4</sup>*Evosep, Odense, Denmark*
- TP 741 **Refining data acquisition parameters for low concentration proteomics using a Vanquish™ Neo LC coupled to an Orbitrap Eclipse™ Mass Spectrometer;** Theodore R. Keppel<sup>1</sup>; Yu Zhou<sup>1</sup>; Jakub Baudys<sup>1</sup>; Dongxia Wang<sup>1</sup>; John R. Barr<sup>1</sup>; <sup>1</sup>*CDC, Atlanta, GA*
- TP 742 **High-throughput Workflow for Deep Analysis of Human Serum Proteome by Mass Spectrometry;** Yanyan Qu<sup>1</sup>; Ravi Tharakan<sup>1</sup>; Yuhong Fang<sup>1</sup>; Claire Weber<sup>2</sup>; Emily Chew<sup>2</sup>; Christopher A LeClair<sup>1</sup>; Dingyin Tao<sup>1</sup>; <sup>1</sup>*National Center for*

## TUESDAY POSTERS

- Advancing Translational Sciences, NIH, Rockville, MD; <sup>2</sup>National Eye Institute, NIH, Bethesda, MD
- TP 743 **Development of a Thiol Exchange- and Mass Spectrometry-Based Proteomic Method for the Evaluation of Protein Folding Kinetics;** Yueqi Chen<sup>1</sup>; Terrence G. Oas<sup>1</sup>; Michael C. Fitzgerald<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC
- TP 744 **High Throughput Abundant Protein Depletion for Plasma Proteomics;** Amarjeet Flora<sup>1</sup>; Anastasia Klenke<sup>1</sup>; Bhavin Patel<sup>1</sup>; Ryan Bomgardner<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, ROCKFORD, IL
- TP 745 **An EasyPep Magnetic solution for automated proteomics sample preparation;** Maowei Dou<sup>1</sup>; Erum Raja<sup>1</sup>; Leigh Foster<sup>1</sup>; Kevin Yang<sup>2</sup>; Amirmansoor Hakimi<sup>2</sup>; Sergei Snovida<sup>1</sup>; Kay Opperman<sup>1</sup>; Bhavin Patel<sup>1</sup>; Ryan Bomgardner<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Rockford, IL; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- TP 746 **Multicolumn Nanoflow Liquid Chromatography System with Accelerated Offline Gradient Generation for Robust and Sensitive Single-Cell Proteome Profiling;** Xiaofeng Xie<sup>1</sup>; Thy Truong<sup>1</sup>; Ryan T. Kelly<sup>1</sup>; Siqi Huang<sup>1</sup>; Madi Johnston<sup>1</sup>; Kei Webber<sup>1</sup>; Lavender Lin<sup>1</sup>; <sup>1</sup>Brigham Young University, Provo, UT
- TP 747 **Proximity Extension Assay-based profiling for candidate biomarker identification in multiple myeloma plasma and comparative evaluation with DIA-MS for cell lysates;** D. R. Mani<sup>1</sup>; Elizabeth D. Lightbody<sup>2</sup>; Kirsty Wienand<sup>1</sup>; Hasmik Keshishian<sup>1</sup>; John Thorup<sup>1</sup>; Simone Zhang<sup>1</sup>; Moe Haines<sup>1</sup>; Shankha Satpathy<sup>1</sup>; Francisca Vazquez<sup>1</sup>; Irene M. Ghobrial<sup>2</sup>; Michael A. Gillette<sup>1</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>Broad Institute, Cambridge, MA; <sup>2</sup>Dana-Farber Cancer Institute, Boston, MA
- TP 748 **Next-generation protein sequencing integrates with top-down and individual ion mass spectrometry to distinguish native and artifactual proteoforms;** Andrew Lee<sup>1</sup>; Kenneth Skinner<sup>2</sup>; Taojunfeng Su<sup>1</sup>; Michael Warchol<sup>2</sup>; Aniel Sanchez<sup>1</sup>; Haidong Huang<sup>2</sup>; Troy D Fisher<sup>1</sup>; Eleonora Forte<sup>1</sup>; Michael A Caldwell<sup>1</sup>; Neil L Kelleher<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Quantum-Si Inc., Branford, CT
- TP 749 **Exploring Digestion Enzymes for Online Microdroplet-Enabled Analysis of LC Separated mAbs;** Timothy Yaroshuk<sup>1</sup>; Andrew Schladebeck<sup>1, 2</sup>; Jim Lau<sup>3</sup>; Mike Knierman<sup>3</sup>; Harsha Gunawardena<sup>4</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>New Jersey Institute of Technology, Newark, NJ; <sup>2</sup>Kenvue, Skillman, NJ; <sup>3</sup>Agilent Technologies, Santa Clara, CA; <sup>4</sup>Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania
- TP 750 **Improved Workflow for Global Comparative Proteomics by LC-MS/MS After Automated High-pH Reversed-Phase Peptide Fractionation Using Solid-Phase Extraction Cartridges;** Debasish Ghosh<sup>1</sup>; Khadiza Zaman<sup>2</sup>; Karsten Liegmann<sup>3</sup>; Brian Shofran<sup>3</sup>; Laszlo Prokai<sup>2</sup>; Vladimir Shulaev<sup>1</sup>; <sup>1</sup>University of North Texas, Denton, TX; <sup>2</sup>University of North Texas Health Science Center, Department of Pharmacology and Neuroscience, Fort Worth, Texas; <sup>3</sup>Tecan, Baldwin Park, CA
- TP 751 **Advancing Model Organism Plasma/Serum Proteomics with Proteograph XT: A species agnostic platform for deep unbiased proteomics profiling;** Shao-Yung Chen<sup>1</sup>; Wei Jiang<sup>2</sup>; Pierre Mbarushimana<sup>2</sup>; Alexis Jacob<sup>2</sup>; Maedeh Zamani<sup>2</sup>; Ryan Hill<sup>2</sup>; Alexey Stukalov<sup>2</sup>; Xiaoyuan Zhou<sup>2</sup>; Ambika Sundaresan<sup>2</sup>; Dashyanng Kachru<sup>2</sup>; Ryan W. Benz<sup>2</sup>; Aaron Gajadhar<sup>2</sup>; <sup>1</sup>Seer, Redwood City, CA; <sup>2</sup>Seer, Inc., Redwood City, CA
- TP 752 **Analysis of the workflow involving protein capture using hydrophilic magnetic beads;** Michael Rosenblatt<sup>1</sup>; Chris Hosfield<sup>1</sup>; Zhiyang Zeng<sup>2</sup>; Wenhui Zhou<sup>2</sup>; Marjeta Urh<sup>1</sup>; <sup>1</sup>Promega Corp, Madison, WI; <sup>2</sup>Promega Corporation, San Luis Obispo, CA
- TP 753 **Characterization of a new ultra-selective, highly active Arginine-C protease for MS-based proteomics;** Tim Heymann<sup>1</sup>; Chris Hosfield<sup>2</sup>; Mike Rosenblatt<sup>2</sup>; Marjeta Urh<sup>2</sup>; Georg Wallmann<sup>1</sup>; Marta Murgia<sup>1</sup>; Matthias Mann<sup>1, 3</sup>; <sup>1</sup>Max Planck Institute of Biochemistry, Martinsried, Germany; <sup>2</sup>Promega Corporation, Madison, WI 53711; <sup>3</sup>Novo Nordisk Foundation Center for Protein Research (CPR), University of Copenhagen, Copenhagen, Denmark
- TP 754 **Chemical acetylation strategy to access previously unidentified ubiquitination sites in lysine-rich regions of the proteome;** Daryl N. Bulloch<sup>1</sup>; Ishwar Kohale<sup>1</sup>; Han-Yin Yang<sup>1</sup>; Kibeom Kim<sup>1</sup>; Aman Makaju<sup>2</sup>; Matthew J. Rardin<sup>1</sup>; <sup>1</sup>Amgen, South San Francisco, CA; <sup>2</sup>Amgen, Thousand Oaks, CA

### SINGLE CELL MS II 755-773

- TP 755 **Massively parallel sample preparation for multiplexed single-cell proteomics using nPOP;** Andrew Leduc<sup>1</sup>; Luke Khoury<sup>1</sup>; Joshua Cantlon<sup>2</sup>; Saad Khan<sup>1</sup>; Nikolai Slavov<sup>1, 3</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Sciencion US, Tempe, AZ; <sup>3</sup>Parallel Squared Technology Institute, Watertown, MA
- TP 756 **Improving multiplexed single-cell proteomics through the combination of Salud real-time prediction and MSFragger-RTS;** Tommy K. Cheung<sup>1</sup>; Fengchao Yu<sup>2</sup>; Alexey I Nesvizhskii<sup>3</sup>; Christopher Rose<sup>4</sup>; <sup>1</sup>Genentech, Inc., South San Francisco, CA; <sup>2</sup>University of Michigan, Ann Arbor, MI; <sup>3</sup>University of Michigan, Ann Arbor, Michigan; <sup>4</sup>Genentech Inc., South San Francisco, CA
- TP 757 **A Tailored Data Handling Workflow for Metabolite Profiling of Single Cells;** Felix Friedrich<sup>1</sup>; Cátia Marques<sup>1</sup>; Ingela Lanekoff<sup>1</sup>; <sup>1</sup>Department of Chemistry – BMC, Uppsala University, Uppsala, Sweden
- TP 758 **Optimizing sample substrates for single-cell metabolomics analysis;** Eszter Szombati<sup>1</sup>; Ingela Lanekoff<sup>1</sup>; <sup>1</sup>Department of Chemistry – BMC, Uppsala University, Uppsala, Sweden
- TP 759 **Unveiling Cellular Secrets: Mass Spectrometry Based Single-Cell Proteomic Analysis of Tissue samples from Familial Adenomatous Polyposis;** Ruiqi Jian<sup>1</sup>; Lihua Jiang<sup>1</sup>; Chenchen Zhu<sup>1</sup>; Tiffany Trinh<sup>1</sup>; Michael P. Snyder<sup>1</sup>; <sup>1</sup>Department of Genetics, Stanford University School of Medicine, Stanford, CA
- TP 760 **Evotip meets the Uno – a transfer-free single cell proteomics approach;** Sibylle Pfammatter<sup>1</sup>; Rafaela Truffer<sup>2</sup>; Ralph Schlapbach<sup>1</sup>; Paolo Nanni<sup>1</sup>; <sup>1</sup>Functional Genomics Center Zurich ETHZ/UZH, Zürich, Switzerland; <sup>2</sup>TECAN Group, Männedorf, Switzerland
- TP 761 **Live single cell mass spectrometry integration with Raman spectroscopy for drug screening;** Congrou Zhang<sup>1</sup>; Arno Germond<sup>2</sup>; Sylvia Le Dévédec<sup>1</sup>; Thomas Hankemeier<sup>1</sup>; Ahmed Ali<sup>1</sup>; <sup>1</sup>Leiden Academic Centre for Drug Research, Leiden University, Leiden, Netherlands; <sup>2</sup>INRAE Centre Clermont-Auvergne-Rhône-Alpes, St Genès Champanelle, France
- TP 762 **Scalable Sample Preparation Workflow for Single Cell Proteomics;** Jing Wang<sup>1</sup>; Olanrewaju Awoyemi<sup>1</sup>; Herbi Yuliantoro<sup>1</sup>; Stephen J Valentine<sup>1</sup>; Peng Li<sup>1</sup>; <sup>1</sup>West Virginia University, Morgantown, WV
- TP 763 **Towards top-down proteomic analysis of limited samples and single cells using porous layer open tubular columns;** Michal Gregus<sup>1</sup>; Yunfan Gao<sup>1</sup>; Anne-Lise Marie<sup>1</sup>; Somak Ray<sup>1</sup>; Alexander R. Ivanov<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA
- TP 764 **Enhancing Sensitivity and Throughput for Low-Input Proteomics: Impact of Tip Integration, Column Length, and Sub-50 µm Internal Diameter Columns;** Thy Truong<sup>1, 2</sup>; Siqi Huang<sup>1</sup>; Xiaofeng Xie<sup>1, 2</sup>; Ryan T. Kelly<sup>1, 2</sup>; <sup>1</sup>Brigham Young University, Provo, UT; <sup>2</sup>MicrOmics Technologies, Spanish Fork, UT
- TP 765 **Single-cell Exploration of Drosophila Oogenesis Identifies Key Actin Regulators;** Merin M Rixen<sup>1</sup>; Joseph A. Loo<sup>2</sup>; Margot E. Quinlan<sup>3</sup>; Rachel Loo<sup>2</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>UCLA, Los Angeles; <sup>3</sup>UCLA, Los Angeles, California
- TP 766 **Automated Single Cell Lipidomics for Mapping MSC Heterogeneity;** Alexandria R Van Grouw<sup>1</sup>; Samuel M

## TUESDAY POSTERS

- TP 767 Erlich<sup>1</sup>; Alexandre E Dunnum<sup>1</sup>; Joseph L Corstvet<sup>1</sup>; Samuel G. Moore<sup>1</sup>; Johnna S Temenoff<sup>1</sup>; Craig R Forest<sup>1</sup>; Facundo M Fernández<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA  
**High-efficiency dual-LIT miniature mass spectrometer enables single-cell lipidomics at high structural specificity**; Zhijun Cai<sup>1</sup>; Ningxi Li<sup>1</sup>; Siming Cheng<sup>1</sup>; Xiaoxiao Ma<sup>1</sup>; Zheng Ouyang<sup>1</sup>; <sup>1</sup>Tsinghua, Beijing, China
- TP 768 **The Good and The Bad of Single-Cell Proteomics by the Most Sensitive Mass Spectrometers - Early Mouse Embryos as Example**; Mo Hu<sup>1</sup>; Yuan Yuan<sup>2</sup>; Yinghui Zheng<sup>2</sup>; Xiaoliang Sunney Xie<sup>1, 2</sup>; <sup>1</sup>Beijing Changping Laboratory, Beijing, China; <sup>2</sup>Peking University, Beijing, China
- TP 769 **Significant impact of laboratory consumable surfaces and sample preparation buffer composition for low-cell number or single-cell proteomics**; Christopher Kune<sup>1</sup>; Sylvia Tielens<sup>2</sup>; Maximilien Fléron<sup>3</sup>; Dominique Baiwir<sup>3</sup>; Denis Vandormael<sup>4</sup>; Laurent Nguyen<sup>2</sup>; Gauthier Eppe<sup>1</sup>; Gabriel Mazzucchelli<sup>1, 3</sup>; <sup>1</sup>Mass Spectrometry Laboratory, MolSys Research Unit, University of Liege, Liege, Belgium; <sup>2</sup>Laboratory of Molecular Regulation of Neurogenesis, GIGA-Stem Cells, University of Liège, Liège, Belgium; <sup>3</sup>GIGA Proteomics Facility, University of Liège, Liège, Belgium; <sup>4</sup>Sirris, Liege, Belgium
- TP 770 **Single-cell metabolomics and lipidomics reveal increased diversity and sub-populations in senescent cells**; Catia Marques<sup>1</sup>; Felix Friedrich<sup>1</sup>; Francesca Castoldi<sup>2</sup>; Federico Pietrocola<sup>2</sup>; Ingela Lanekoff<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>Karolinska Institutet, Solna, Sweden
- TP 771 **Liquid chromatography coupled to untargeted lipidomics of single-cells with fluorescent live cell imaging of lipid droplets**; Johanna Von Gerichten<sup>1</sup>; Kyle D.G. Saunders<sup>1</sup>; Anthony D. Whetton<sup>2</sup>; Melanie Bailey<sup>1</sup>; <sup>1</sup>University of Surrey, School of Chemistry and Chemical Engineering, Guildford, United Kingdom; <sup>2</sup>vHive, School of Veterinary Medicine, School of Biosciences and Medicine, University of Surrey, Guildford, United Kingdom
- TP 772 **Novel Nanoliter-Volume Sample Injection Technique Enables Top-down Proteomic and N-glycomics CE-MS-Based Profiling of Single Cells**; Yunfan Gao<sup>1</sup>; Michal Gregus<sup>1</sup>; Anne-Lise Marie<sup>1</sup>; Alexander R. Ivanov<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA
- TP 773 **An open source autosampler for trace proteomics of tissue samples**; Nathaniel B Axtell<sup>1</sup>; Kei Webber<sup>1</sup>; Siqi Huang<sup>1</sup>; Tarah Gudmundson<sup>1</sup>; Ryan T Kelly<sup>1</sup>; <sup>1</sup>BYU, Provo, UT
- SMALL MOLECULES: QUALITATIVE AND QUANTITATIVE ANALYSIS II**  
774-794
- TP 774 **Explanation for Discrepancies in Quantitative Mass Spectrometric Analysis of RNA Modifications**; Frank Morales Shnaider; university of north carolina greensboro, Greensboro, NC
- TP 775 **Repeated Analysis including Incurred Sample Re-assay (ISR) for Ivermectin and Praziquantel Bioequivalence (BE) Study using Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS)**; Linge (Emily) Li<sup>1</sup>; Karyn D. Howard<sup>1</sup>; Michael J. Myers<sup>1</sup>; <sup>1</sup>FDA/CVM, Laurel, MD
- TP 776 **Development of a sensitive and high-throughput UPLC-MS/MS method for the quantification of multiple antiretrovirals in human tissues**; Raymond E. West III<sup>1</sup>; Patrick J. Oberly<sup>1</sup>; Thomas D. Nolin<sup>1</sup>; Aaron S. Devanathan<sup>1</sup>; <sup>1</sup>University of Pittsburgh, Pittsburgh, PA
- TP 777 **Development and Validation of a Simple and Rugged LC-MS/MS Method to Measure Amifampridine and N-Acetyl-Amifampridine in Human Plasma**; Nick Peng<sup>1</sup>; Jayce Brown<sup>1</sup>; Ardeshir Khadang<sup>1</sup>; <sup>1</sup>Axis Clinicals, Dilworth, MN
- TP 778 **Characterization of new psychoactive substances using high resolution mass spectrometry structural assignment software**; Alan Barnes<sup>1</sup>; Peter Schein<sup>2</sup>; David I Dixon<sup>3</sup>; Molly F Millea<sup>3</sup>; Emily G Armitage<sup>1</sup>; Ben Barrett<sup>4</sup>; Ryan E Mewis<sup>3</sup>; Oliver B Sutcliffe<sup>3</sup>; Neil J Loftus<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Manchester, United Kingdom; <sup>2</sup>Shimadzu Deutschland GmbH, Duisburg, Germany; <sup>3</sup>MANchester DRug Analysis and Knowledge Exchange (MANDRAKE), Manchester Metropolitan University, Manchester, United Kingdom; <sup>4</sup>Shimadzu UK Limited, Milton Keynes, United Kingdom
- TP 779 **Development of Highly Sensitive Bioanalytical Methods for Peptide Based Therapeutics**; Xiaodong Zhu<sup>1</sup>; Steven Hoehne<sup>1</sup>; Jingguo Hou<sup>1</sup>; Xiaomei Bian<sup>1</sup>; Leimin Fan<sup>1</sup>; <sup>1</sup>Worldwide Clinical Trials, Austin, TX
- TP 780 **A Sensitive 2D-LC/MS/MS Method with a Novel Derivatization for the Quantitation of delta-9-tetrahydrocannabinol, 11-Hydroxy-delta-9-THC and 11-nor-9-Carboxy-delta-9-THC in Human Plasma**; Jingduan Chi<sup>1</sup>; Melissa Mofikoya<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific Inc, Madison, WI; <sup>2</sup>Thermo Fisher Scientific Inc., Madison, WI
- TP 781 **Analysis of Ibuprofen and Three Modulator Drugs of Cystic Fibrosis Triple Combination Therapy in Human Plasma by LC-MS/MS**; Xiaolin Li<sup>1</sup>; Daniela M. Schlatter<sup>1</sup>; Tracey L. Bonfield<sup>1</sup>; Mark R. Chance<sup>2</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>Case Western Reserve University, Cleveland, Ohio
- TP 782 **Comprehensive characterization of phytosiderophore-metal complexes with LC-QTOFMS and IM-MS**; Andreea Spiridon<sup>1</sup>; Eva Oburger<sup>1</sup>; Tim Causon<sup>1</sup>; Stephan Hann<sup>1</sup>; <sup>1</sup>University of Natural Resources and Life Sciences, Vienna, Austria
- TP 783 **Sensitive and selective quantitation of bimatoprost in human plasma using accurate mass spectrometry**; Ian Moore<sup>1</sup>; Sujata Rajan<sup>2</sup>; Rahul Baghla<sup>3</sup>; Eshani Galermo<sup>3</sup>; <sup>1</sup>SCIEX, Framingham; <sup>2</sup>SCIEX, Bangalore, India; <sup>3</sup>SCIEX, Redwood City, CA
- TP 784 **Redefining bioanalysis: assessment of a mass spectrometer robustness versus complex matrix**; Elliott Jones<sup>1</sup>; Rahul Baghla<sup>1</sup>; Ebru Selen<sup>1</sup>; Ian Moore<sup>2</sup>; Eshani Galermo<sup>1</sup>; <sup>1</sup>SCIEX, Redwood City, CA; <sup>2</sup>SCIEX, Framingham
- TP 785 **A LC-MS/MS Method for the Determination of the Near-infrared Fluorescence-targeted Contrast Agent in in-vitro Hepatocytes Metabolic Stability Assay**; Ruolan Yang<sup>1</sup>; Dan Li<sup>1</sup>; Yangzhen Zheng<sup>1</sup>; Jinlian Lu<sup>1</sup>; Zhiyu Li<sup>1</sup>; Lili Xing<sup>1</sup>; Yi Tao<sup>1</sup>; Liang Shen<sup>1</sup>; <sup>1</sup>WuXi AppTec, Shanghai, China
- TP 786 **Sensitive quantitative LC-MS/MS method of steroid hormones determination in adipose tissue as a helpful tool in obesity research**; Rafal Szewczyk<sup>1, 2</sup>; Anna Lenartowicz<sup>1</sup>; Alina Kurylowicz<sup>3</sup>; Katarzyna Krupczyńska-Stopa<sup>1, 2</sup>; Maciej Stopa<sup>1, 2</sup>; <sup>1</sup>LabExperts sp z o.o., Gdańsk, Poland; <sup>2</sup>Bioanalytic sp z o.o., Gdańsk, Poland; <sup>3</sup>Department of Human Epigenetics, Mossakowski Medical Research Centre, Polish Academy of Sciences, Warsaw, Poland
- TP 787 **A Novel Microliter Volume Injection System Based on the High Contact Angle Pinning Phenomena for High-Throughput MS**; Nate Hoxie<sup>1</sup>; Jenna Miller<sup>1</sup>; Vijay Veerisetty<sup>1</sup>; Meghav Verma<sup>1</sup>; John Janiszewski<sup>1</sup>; Jonathan Shrimp<sup>1</sup>; Bolormaa Baljinnyam<sup>1</sup>; Michael Ronzetti<sup>1</sup>; Peter Kovarik<sup>2</sup>; Tom Covey<sup>2</sup>; Chang Liu<sup>2</sup>; Richard B van Breemen<sup>3</sup>; Gary J Van Berkel<sup>4</sup>; Sam Michael<sup>1</sup>; Anton Simeonov<sup>1</sup>; Matthew D Hall<sup>1</sup>; Savannah Wood<sup>1</sup>; <sup>1</sup>National Center for Advancing Translational Sciences, NIH, Rockville, MD; <sup>2</sup>SCIEX, Concord, ON; <sup>3</sup>Linus Pauling Institute, Oregon State University, Corvallis, OR; <sup>4</sup>Van Berkel Ventures, LLC., Oak Ridge, TN
- TP 788 **UHPLC-tandem MS quantitation of Quorum Sensing molecules in plasma samples of patients with AKI (Acute Kidney Injury) in sub-intensive care**; Alex Affricano<sup>1</sup>; Vito Fanelli<sup>1</sup>; Vincenzo Cantaluppi<sup>2</sup>; Claudio Medana<sup>1</sup>; Federica Dal Bello<sup>1</sup>; <sup>1</sup>University of Turin, Torino, Italy; <sup>2</sup>University of Eastern Piedmont, Novara, Italy
- TP 789 **Toward a predictive model of the optimal supported liquid extraction (SLE) strategies for small molecule bioanalysis by LC-MS/MS**; Yuxiang Cui<sup>1</sup>; Xiaorong Liang<sup>1</sup>; Brian Dean<sup>1</sup>; Liuxi Chen<sup>1</sup>; <sup>1</sup>Genentech Inc, South San Francisco, CA

## TUESDAY POSTERS

- TP 790 **Simultaneous Quantitation and Discovery (SQUAD) Metabolomics Workflow on the Orbitrap IQ-X for the Analysis of Fecal Bile Acids;** Allison Stewart<sup>1</sup>; Bashar Amer<sup>2</sup>; Rahul Deshpande<sup>1</sup>; Andrew Percy<sup>3</sup>; Krista Backiel<sup>3</sup>; Joshua P. Kline<sup>2</sup>; Brandon Bills<sup>2</sup>; Susan Bird<sup>2</sup>; <sup>1</sup>*ThermoFisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*Cambridge Isotope Laboratories, Tewksbury, Massachusetts*
- TP 791 **Detection, quantification, and confirmation of 14 compounds affecting hypoxia-inducible factor in equine plasma and urine by LC-HRMS;** Matthew A. Adreance<sup>1,2</sup>; Fuyu Guan<sup>1,2</sup>; Savannah Fay<sup>1,2</sup>; Mary A. Robinson<sup>1,2</sup>; <sup>1</sup>*Department of Clinical Studies – New Bolton Center, School of Veterinary Medicine, University of Pennsylvania, Kennett Square, PA*; <sup>2</sup>*Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA*
- TP 792 **Quantification of Sirolimus in Equine Whole Blood by UHPLC-MS/MS;** Jaclyn R. Missanelli<sup>1,2</sup>; Youwen You<sup>1,2</sup>; Rachel M. Proctor<sup>1,2</sup>; Andrew Van Eps<sup>1</sup>; Joanne Haughan<sup>1</sup>; Mary A. Robinson<sup>1,2</sup>; <sup>1</sup>*University of Pennsylvania School of Veterinary Medicine, Pennsylvania, PA*; <sup>2</sup>*Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA*
- TP 793 **Rapid and Sensitive detection of enantiomeric D- and L-Lactae in cancer cell Using High-performance Liquid Chromatography-Negative Electropray Mass Spectrometry;** Liangqiao Bian<sup>1</sup>; Raj Ritu<sup>2</sup>; Eul Hyun Suh<sup>2</sup>; <sup>1</sup>*SCAAC, UT Arlington, Arlington, TX*; <sup>2</sup>*Department of Pharmaceutical Sciences, UNT System College of Pharmacy, University of North Texas Health Science Center, Fort Worth, TX*
- TP 794 **Rapid, Sensitive and Direct Quantitation of Tiotropium at sub-pg/mL in Plasma using Shimadzu LCMS-8060NX;** Yogesh G Arote<sup>1</sup>; Avinash B Gaikwad<sup>1</sup>; Chaitanya Krishna A<sup>1</sup>; <sup>1</sup>*ADC-Shimadzu Analytical India Pvt Ltd, NAVI MUMBAI, India*
- STABLE ISOTOPE LABELING**  
795-809
- TP 795 **SLC45A4 encodes a mitochondrial transporter that promotes GABA synthesis from ornithine;** Cecilia Colson<sup>1</sup>; James Atherton<sup>1</sup>; Yujue Wang<sup>1</sup>; Xiaoyang Su<sup>1</sup>; <sup>1</sup>*Rutgers University- New Brunsw, New Brunswick, NJ*
- TP 796 **Monitoring de novo Biosynthesis of Amino Acids with 13C-labeled Glucose;** Simpson Jeffrey<sup>1</sup>; Eric M George<sup>2</sup>; Greenwalt Scott<sup>1</sup>; Heather Platt<sup>1</sup>; Suresh Annangudi<sup>1</sup>; <sup>1</sup>*Corteva Agriscience, Indianapolis, IN*; <sup>2</sup>*Purdue University, West Lafayette, IN*
- TP 797 **ClickZip: ultra-stable lanthanide mass tags for multiplex assay;** Tomáš David<sup>1</sup>; Miroslava Šedinová<sup>1</sup>; Aneta Myšková<sup>1,2</sup>; Ibrahim Demirci<sup>1</sup>; Jiří Böserle<sup>1</sup>; Helena Mertlíková Kaiserová<sup>1</sup>; Miroslava Litecká<sup>3</sup>; Blanka Klepetářová<sup>1</sup>; Karel Čížek<sup>1</sup>; Lenka Maletínská<sup>1</sup>; Miloslav Polasek<sup>1</sup>; <sup>1</sup>*Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic*; <sup>2</sup>*University of Chemistry and Technology Prague, Prague, Czech Republic*; <sup>3</sup>*Institute of Inorganic Chemistry of the CAS, Husinec-Řež, Czech Republic*
- TP 798 **Metabolomic comparison between hepatic fibrosis and pulmonary fibrosis using 13C-MFA(Metabolic Flux Analysis);** Mi Jeong Kim<sup>1</sup>; Ha Eun SONG<sup>1</sup>; Hyun Ju Yoo<sup>1</sup>; <sup>1</sup>*ASAN Medical center, SEOUL, South Korea*
- TP 799 **Discovering mode of action of novel compounds through nascent proteome analysis: Bostrycin induces cell death via ferroptotic pathways;** Lina-Marie Wagner<sup>1</sup>; Syed A. Ali<sup>1</sup>; Isabelle Becher<sup>2</sup>; Mira Burtscher<sup>2</sup>; Mikhail Savitski<sup>2</sup>; Jeroen Krijgsveld<sup>1,3</sup>; <sup>1</sup>*German Cancer Research Center, Heidelberg, Germany*; <sup>2</sup>*EMBL, Heidelberg, Germany*; <sup>3</sup>*Heidelberg University, Medical Faculty, Heidelberg, Germany*
- TP 800 **14-plex DeAla Isobaric Reagents for High-Throughput Proteome-wide Quantification;** Peng-Kai Liu<sup>1</sup>; Ting-Jia Gu<sup>2</sup>; Danqing Wang<sup>3</sup>; Lingjun Li<sup>1,2,3</sup>; <sup>1</sup>*Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI*; <sup>2</sup>*School of Pharmacy, University of Wisconsin-Madison, Madison, WI*; <sup>3</sup>*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*
- TP 801 **Sulfur-34 labeling of a thiophosphoramidate-containing cyclic dinucleotide for use as an internal standard in LC-MS quantification of a STING agonist;** Michael A Wallace<sup>1</sup>; Alban J Allentoff<sup>1</sup>; Sharon X Gong<sup>1</sup>; Samuel Bonacorsi, Jr. <sup>1</sup>; Jim X Shen<sup>1</sup>; Felicia Dunsmuir<sup>2</sup>; Daniel Bennett<sup>2</sup>; <sup>1</sup>*Bristol Myers Squibb, Princeton, NJ*; <sup>2</sup>*Syneos Health, Somerset, New Jersey*
- TP 802 **Application of tandem mass tag labeling to understand virus resistance to free chlorine;** Chonglin Zhu<sup>1</sup>; Yinyin Ye<sup>1</sup>; <sup>1</sup>*University at Buffalo, Buffalo, NY*
- TP 803 **Metabolic pulse-chase multiplex proteomics reveals impaired protein turnover in aging brain is due to reduced turnover of proteolytic proteasome subunits;** Jeffrey N Savas<sup>1</sup>; Nalini R. Rao<sup>2</sup>; Arun Upadhyay<sup>2</sup>; <sup>1</sup>*Northwestern University, Feinberg School of Medicine, Chicago, IL*; <sup>2</sup>*Northwestern University Feinberg School of Medicine, Chicago, IL*
- TP 804 **Stable Isotope Resolved Metabolomics of cancer cells by Cation-Exchange Ion Chromatography Coupled to Ultra-High Resolution Mass Spectrometry;** Mohamed M. Y. Kaddah<sup>1</sup>; Teresa Fan<sup>1</sup>; Andrew Lane<sup>1</sup>; Richard Higashi<sup>1</sup>; <sup>1</sup>*University of Kentucky, Lexington, KY*
- TP 805 **24-plex high throughput quantitation of carboxylic acid metabolites for pharmaceutical dose response curves.;** BRIANA Mwinkom TENGAN<sup>1</sup>; Micheal Armbruster<sup>2</sup>; James Edwards<sup>2</sup>; <sup>1</sup>*Saint Louis University, Saint Louis, MO*; <sup>2</sup>*SAINT LOUIS UNIVERSITY, St Louis, MO*
- TP 806 **18O-water labelling enables protein turnover measurements in embryogenesis.;** Edward R Cruz<sup>1</sup>; Argit Marishta<sup>1</sup>; Alex Johnson<sup>1</sup>; Aleigha Reynolds<sup>1</sup>; Michael Neinast<sup>1</sup>; Joseph Crapse<sup>1</sup>; Joshua D. Rabinowitz<sup>1</sup>; Eric F. Wieschaus<sup>1</sup>; Martin Wuhr<sup>1</sup>; <sup>1</sup>*Princeton University, Princeton, NJ*
- TP 807 **Analytical solution for dynamic label incorporation in atom-based metabolic labeling;** Henock Deberneh<sup>1</sup>; Rovshan Sadygov<sup>2</sup>; <sup>1</sup>*The University of Texas Medical Branch, Galveston, TX*; <sup>2</sup>*University of Texas Medical Branch, Galveston, TX*
- TP 808 **A 23rd proteogenic amino acid? The Hidden Homoarginine Proteome Revealed Using a Novel Activity-based Arginylation Profiling Platform;** Daniel H Ramirez<sup>1</sup>; Zongtao Lin<sup>1</sup>; Benjamin A Garcia<sup>1</sup>; <sup>1</sup>*Washington University in St. Louis, St. Louis, MO*
- TP 809 **A comprehensive protein turnover atlas for drug discovery;** Goetz Hagemann<sup>1</sup>; Barbara Schnitzer<sup>1</sup>; Leonie Reichert<sup>1</sup>; Alexander Betz<sup>1</sup>; Christin Zasada<sup>1</sup>; Hannes Hahne<sup>1</sup>; <sup>1</sup>*OmicScouts GmbH, Freising, Germany*

## WEDNESDAY POSTERS

### WEDNESDAY POSTERS

Set up all Wednesday posters  
6:30 - 9:00 am

**Odd-numbered posters present**  
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

**Even-numbered posters present**  
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Wednesday posters  
5:00 - 8:00 pm

Ambient Ionization: Fundamentals and Instrumentation .....	001-008
Antibodies & Antibody Drug Conjugates .....	009-039
Artificial Intelligence in MS Instrumentation .....	040-064
Biomarkers: Discovery I .....	065-101
Biomarkers: Quantitative Analysis II .....	102-127
Cancer Research I .....	128-165
Clinical Analysis I .....	166-196
Covalent Labeling and Chemical Crosslinking .....	197-222
Drug Discovery: Qualitative and Quantitative .....	223-247
Environmental: General III .....	248-284
Fundamentals: Unconventional Approaches in MS .....	285-293
Glycoproteins I .....	294-324
High Throughput MS II .....	325-349
Imaging MS: Method Development I .....	350-383
Informatics: Protein ID and Quantification .....	384-396
Informatics: Workflow and Data Management .....	397-430
Instrumentation: Mini/Portable/Fieldable MS .....	431-442
Instrumentation: New Developments in Mass .....	443-458
Ion Mobility: FAIMS/DMS .....	459-465
Ion Mobility: General .....	466-479
LC/MS: Chromatography and Software .....	480-492
LC/MS: Sample Preparation II .....	493-512
Metabolomics: Targeted and Quantitative Analysis .....	513-533
Neuroscience and Neurodegenerative Disease Research II .....	534-558
Nucleic Acids and Oligonucleotides III .....	559-585
Peptides: Targeted and Quantitative Analysis .....	586-616
Protein Therapeutics: Quantitative Analysis .....	617-641
Proteins: General and Membrane .....	642-657
Proteins: PTMs I .....	658-677
Proteomics: Intact Proteins and Top .....	678-708
Proteomics: Quantitative I .....	709-743
Proteomics: Tissue .....	744-772
Single Cell MS III .....	773-794
Synthetic Polymers .....	795-808
Toxicology .....	809-821

### AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION 001-008

- WP 001 **Rapid Fabrication of Hydrophobic/Hydrophilic Patterns on Paper Substrates for Paper Spray Mass Spectrometry;** Peyton Windham<sup>1</sup>; Austin Arias<sup>1</sup>; Mac Gilliland<sup>1</sup>; <sup>1</sup>*Furman University, Greenville, SC*
- WP 002 **Solvent-Assisted Laser Desorption Coupled to Flexible Microtube Plasma Mass Spectrometry for the Analysis of Samples Deposited on Paper;** Marcos Bouza Areces<sup>1</sup>; Norman Ahlmann<sup>2</sup>; Juan F. Gracia-Reyes<sup>1</sup>; Joachim Franzke<sup>2</sup>; <sup>1</sup>*University of Jaén, Jaén, Spain*; <sup>2</sup>*Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., Dortmund, Germany*
- WP 003 **Influence of Inlet Capillary Parameters on the Ion Signals of Species Analyzed in the AP MALDI source;** Eugene Moskovets<sup>1</sup>; Josie Daldegan Rezende<sup>2</sup>; Jace W. Jones<sup>2</sup>; <sup>1</sup>*MassTech Inc, Columbia, MD*; <sup>2</sup>*School of Pharmacy, University of Maryland, Baltimore, MD*
- WP 004 **Solid phase microextraction coupled direct analysis in real-time mass spectrometry (SPME-DART-MS) for the ignitable liquid residue analysis;** Shruthi Perna<sup>1</sup>; Mengliang Zhang<sup>1</sup>; Ngee Sing Chong<sup>1</sup>; Victoria Bascou<sup>1</sup>; <sup>1</sup>*Middle Tennessee State University, Murfreesboro, TN*
- WP 005 **Understanding Signal Enhancement of Lipids by Fluoride-Containing Additives in Electrospray Ionization;** Emerson Hernly<sup>1</sup>; Aiming Zheng<sup>1</sup>; Syeda Nazifa Wali<sup>1</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>*Purdue University, Department of Chemistry, West Lafayette, IN*
- WP 006 **Ambient Gas Atmosphere Influence on Onset Potential for Electrospray Ionization Mass Spectrometry;** Khadija Khetabi<sup>1</sup>; Amy Le<sup>1</sup>; Andre R. Venter<sup>2</sup>; Richard B. Cole<sup>1, 3</sup>; <sup>1</sup>*Sorbonne Universite - Paris 06, Paris Cedex 05, France*; <sup>2</sup>*Western Michigan University, Kalamazoo, MI*; <sup>3</sup>*University of New Orleans, New Orleans, LA*
- WP 007 **Integrating Mass Spectrometry and Machine Learning for Comprehensive Characterization of Textile Dyes and Fiber Identification;** Jiarui Wu<sup>1</sup>; Nelson Vinueza<sup>1</sup>; <sup>1</sup>*North Carolina State University, Raleigh, NC*
- WP 008 **Laser Printer Printed Ion Sources for Mass Spectrometric Analysis of Polar and Nonpolar Analytes;** Chin-Poa Chiu<sup>1</sup>; Yu-Chie Chen<sup>1</sup>; <sup>1</sup>*National Yang Ming Chiao Tung University, Hsinchu City, Taiwan*

### ANTIBODIES & ANTIBODY DRUG CONJUGATES 009-039

- WP 009 **Decoding mAb Charge Variants: Unveiling Hidden Complexity with Native CE-MS Analysis;** Weihan Wang<sup>1</sup>; Qing Mike Tang<sup>1</sup>; Ping Hu<sup>1</sup>; <sup>1</sup>*Janssen Research & Development, LLC, Malvern, PA*
- WP 010 **An Integrated Strategy to Identify Tyrosine Sulfation/phosphorylation in Therapeutic Proteins;** Eunju Jang<sup>1</sup>; Fengfei Ma<sup>2</sup>; Daniela Tomazela<sup>1</sup>; Laurence Fayadat-Dilman<sup>1</sup>; Mohammad Ahmed Al-Sayah<sup>2</sup>; <sup>1</sup>*Protein Sciences, Discovery Biologics, Merck & Co., Inc., South San Francisco, CA, USA, South San Francisco, California*; <sup>2</sup>*Discovery Analytical Research, Analytical Enabling Capabilities, Merck & Co., Inc., South San Francisco, CA, USA, South San Francisco, California*
- WP 011 **Development of novel chromatography techniques for sensitive mass spectrometry detection of mis-paired and low molecular weight impurities in bispecific antibodies;** Bengian Wei<sup>1</sup>; Fengfei Ma<sup>2</sup>; Daniela Tomazela<sup>3</sup>; Laurence Fayadat-Dilman<sup>3</sup>; <sup>1</sup>*Analytical Research and Development, Merck & Co., Inc., Rahway, NJ*; <sup>2</sup>*Analytical Research and Development, Merck & Co., Inc., South San Francisco, CA*; <sup>3</sup>*Protein Sciences, Discovery Biologics, Merck & Co., Inc., South San Francisco, CA*
- WP 012 **Characterization of a site-specific antibody-drug conjugate using native mass spectrometry and electron activated dissociation-based middle-down workflows;** Haichuan Liu<sup>1</sup>; Elliott Jones<sup>1</sup>; Zoe Zhang<sup>1</sup>; <sup>1</sup>*SCIEX, Redwood City, CA*

## WEDNESDAY POSTERS

- WP 013 **A comprehensive mass-spectrometry approach for de novo protein sequencing of biotherapeutics using multiple fragmentation, proteases, bottom-up and middle-down MS;** Janine Y. Fu<sup>1</sup>; Ashley Yoon<sup>1</sup>; Edward J. Hsieh<sup>1</sup>; Magdeleine Hung<sup>1</sup>; Daniela M. Tomazela<sup>1</sup>; <sup>1</sup>*Gilead Sciences Inc., Foster City, CA*
- WP 014 **Exposing distinctive quantitative traits in structural isomers on Fc-glycans of human IgG subclasses;** Weiwei Wang<sup>1,2</sup>; Joshua Maliepaard<sup>1,2</sup>; Gestur Vidarsson<sup>1,2</sup>; Albert J.R. Heck<sup>1,2</sup>; Karli Reiding<sup>1,2</sup>; <sup>1</sup>*Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht University, Padualaan 8, 3584 CH, Utrecht, Netherlands*; <sup>2</sup>*Netherlands Proteomics Center, Utrecht, Netherlands*
- WP 015 **From Antagonist to Agonist: Exploring the Structural Implications of Antibody Isotype Switching Using Ion Mobility-Mass Spectrometry and Collision-Induced Unfolding;** Rosendo C Villafuerte-Vega<sup>1</sup>; Alyssa Erlenbeck<sup>1</sup>; Hayden Fisher<sup>2</sup>; Isabel Elliot<sup>2</sup>; Mark S Cragg<sup>2</sup>; Brandon T Ruotolo<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, Michigan*; <sup>2</sup>*University of Southampton, Southampton, United Kingdom*
- WP 016 **In-depth structural characterization of the micro-heterogeneity of monoclonal antibodies (mAbs) with improved Fourier Transform Orbitrap mass spectrometry;** Cong Wang<sup>1</sup>; Xiaoxi Zhang<sup>2</sup>; Rafael Melani<sup>3</sup>; Eugen Damoc<sup>1</sup>; Kyle L. Fort<sup>1</sup>; Min Du<sup>4</sup>; Claire Dauly<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Bremen, Germany*; <sup>2</sup>*Thermo Fisher Scientific, Shanghai, China*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>4</sup>*Thermo Fisher Scientific, Remote, MS*
- WP 017 **Detailed characterization of monoclonal antibodies charge variants using capillary electrophoresis and tandem mass spectrometry;** Lola Alez-Martin<sup>1,2</sup>; Pascal Houzé<sup>2</sup>; Rania Joomun<sup>2</sup>; Nathalie Mignet<sup>2</sup>; Yannis-Nicolas François<sup>1</sup>; Rabah Gahoual<sup>2</sup>; <sup>1</sup>*Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, Strasbourg, France*; <sup>2</sup>*Université Paris Cité, Unité de Technologies Chimiques et Biologiques pour la Santé (UTCBS), CNRS UMR8258, Inserm U1022, Faculté des sciences pharmaceutiques et biologiques, Paris, France*
- WP 018 **De novo Sequencing of Polyclonal Antibodies to Identify Functional and Neutralizing Factors in Human Plasma Post-SARS-CoV-2 Vaccination;** Thierry Le Bihan<sup>1</sup>; Teresa Nunez De Villavicencio Diaz<sup>1</sup>; Chelsea Reitzel<sup>1</sup>; Victoria Lange<sup>1</sup>; Minyoung Park<sup>1</sup>; Emma Beadle<sup>1</sup>; Lin Wu<sup>1</sup>; Marko Jovic<sup>1</sup>; Rosalin M. Dubois<sup>1</sup>; Amber L. Couzens<sup>1</sup>; Jin Duan<sup>1</sup>; Xiaobing Han<sup>1</sup>; Qixin Liu<sup>1</sup>; Bin Ma<sup>1</sup>; <sup>1</sup>*Rapid Novor, Kitchener, Ontario*
- WP 019 **Development of an LC-MS/MS Method for Quantifying PGT 121.414.LS in Human Serum;** Connor E Gould<sup>1</sup>; Qing Ma<sup>2</sup>; Raymond Cha<sup>2</sup>; Kevin J Zemaitis<sup>3</sup>; Robin Difrancesco<sup>2</sup>; Gene D. Morse<sup>2</sup>; Troy D. Wood<sup>1,2</sup>; <sup>1</sup>*SUNY at Buffalo, Buffalo, NY*; <sup>2</sup>*Translational Pharmacology Research Core and Global Botanical Sciences Program, Center for Integrated Global Biomedical Sciences, Department of Pharmacy Practice, School of Pharmacy and Pharmaceutical Sciences, University at Buffalo, Buffalo, NY*; <sup>3</sup>*Earth and Biological Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA*
- WP 020 **A High-Throughput, Annotation Agnostic Method for Review, Visualization, and Outlier Detection of Mass Distributions for Therapeutic Proteins;** Patrick Brophy<sup>1</sup>; Mark Benhaim<sup>1</sup>; Nate Joh<sup>1</sup>; <sup>1</sup>*Generate Biomedicines, Somerville, MA*
- WP 021 **Assessment of bioavailability of a low-level VHS variant in biotherapeutic following subcutaneous administration using IA-LC-MS/MS;** Luna Liu<sup>1</sup>; Jim Zanghi<sup>2</sup>; Chang Liu<sup>3</sup>; Michael T Kim<sup>3</sup>; Cynthia Quan<sup>3</sup>; Keyang Xu<sup>3</sup>; <sup>1</sup>*Genentech, Inc., South San Francisco, CA*; <sup>2</sup>*Genentech Inc., South San Francisco, CA*; <sup>3</sup>*Genentech Inc, South San Francisco, CA*
- WP 022 **Improved LC-MS Host Cell Protein Detection in Biologics by Incorporation of New Advances in Sample Preparation and Data-Independent Acquisition;** Daniel Woodall<sup>1</sup>; Jeffrey J Liu<sup>1</sup>; Gang Xiao<sup>1</sup>; Aman Makaju<sup>1</sup>; Pavel V. Bondarenko<sup>1</sup>; <sup>1</sup>*Amgen, Thousand Oaks, CA*
- WP 023 **A novel validated LC-MS/MS approach for simultaneous determination of total antibody and conjugate payload for DS-8201 in SD rat serum;** Zhiren Yu<sup>1</sup>; Hefeng Zhang<sup>1</sup>; Zhiyu Li<sup>1</sup>; Hongmei Wang<sup>1</sup>; Nan Zhao<sup>1</sup>; Lili Xing<sup>1</sup>; Yi Tao<sup>1</sup>; Liang Shen<sup>1</sup>; <sup>1</sup>*WuXi AppTec, Shanghai, China*
- WP 024 **Characterization of Coformulated Therapeutic Proteins by Mass Spectrometry;** Lidong He<sup>1</sup>; Qingchun Zhang<sup>1</sup>; Suminda Hapuarachchi<sup>1</sup>; <sup>1</sup>*Amgen, Thousand Oaks, CA*
- WP 025 **Rapid LC-MS methods to de-risk complex novel biologics using middle-level characterisation: enhancing our early stage research development assessments;** Esther Marie Martin<sup>1</sup>; Kyna Griffiths<sup>1</sup>; Noemi Mallorqui-Fernandez<sup>1</sup>; Stanislas Blein<sup>1</sup>; <sup>1</sup>*AstraZeneca, Cambridge, United Kingdom*
- WP 026 **Size Exclusion Column Considerations for Antibody Drug Conjugates;** Alycia K Uyeoka<sup>1</sup>; Fan Zhang<sup>1</sup>; Esther Kofman<sup>1</sup>; Mehabaw Derebe<sup>1</sup>; Laurence Fayadat-Dilman<sup>1</sup>; Jason Hogan<sup>1</sup>; <sup>1</sup>*Discovery Biologics, Protein Sciences, Merck & Co., Inc., South San Francisco, CA*
- WP 027 **Development of LC/MS Platform Methods for the Characterization of Bispecific Antibodies;** Robert J Schuster<sup>1</sup>; Philip H Yoo<sup>1</sup>; Lana V Fabia<sup>1</sup>; Nicole A Schneck<sup>1</sup>; <sup>1</sup>*GSK, Collegeville, PA*
- WP 028 **Sample preparation and nLC-MS/MS optimization for mAb characterizing;** Rodrigo S C Brant<sup>1</sup>; Kelly Cavalcanti Machado<sup>2</sup>; Thiago Bousquet Bandini<sup>2</sup>; Hulyana Brum<sup>2</sup>; Anna Erika Vieira De Araujo<sup>1</sup>; Iaralice Medeiros De Souza<sup>1</sup>; Michel Batista<sup>2</sup>; <sup>1</sup>*Fiocruz, Curitiba, Brazil*; <sup>2</sup>*Mass Spectrometry Facility, Fiocruz, Curitiba, Brazil*
- WP 029 **Development of a High-Throughput Host Cell Proteomics Method to Support Next Generation Manufacturing of Biopharmaceuticals;** Jake A. Melby<sup>1</sup>; Samik Das<sup>1</sup>; Ken Lee<sup>1</sup>; Wei Xu<sup>1</sup>; Yu Shi<sup>1</sup>; <sup>1</sup>*AstraZeneca, Gaithersburg, MD*
- WP 030 **Monitoring oxidation in recombinant monoclonal antibodies at subunit level through two-dimensional liquid chromatography coupled with mass spectrometry;** Anurag Singh Rathore<sup>1</sup>; Vadiraja B. Bhat<sup>2</sup>; Sunil Kumar<sup>1</sup>; Deepika Sarin<sup>1</sup>; <sup>1</sup>*Indian Institute of Technology Delhi, New Delhi, India*; <sup>2</sup>*Agilent technologies, Bangalore, India*
- WP 031 **Localization and Quantification of Lysine Conjugation by Peptide Mapping;** Amber Peariso<sup>1</sup>; Zhongping Liao<sup>1</sup>; <sup>1</sup>*Eli Lilly and Company, Indianapolis, IN*
- WP 032 **Ubiquitin: Characterization of a Host Cell Protein Covalently Attached to a Monoclonal Antibody Product by LC-MS/MS;** Regina Kufer<sup>1</sup>; Vincent Larraillet<sup>2</sup>; Sabrina Thalhauser<sup>1</sup>; Tobias Graf<sup>1</sup>; Manuel Endesfelder<sup>2</sup>; Stefanie Wohlrab<sup>1</sup>; <sup>1</sup>*Roche Diagnostics GmbH, Penzberg, Germany*; <sup>2</sup>*Roche Pharmaceutical Research and Early Development, Large Molecule Research, Roche Innovation Center Munich, Germany*
- WP 033 **Assessment of different MS Label-Free Quantitation Strategies for Therapeutic Proteins;** Vahid Golghalyani<sup>1</sup>; Eva Vosika<sup>2</sup>; Juergen Fichtl<sup>2</sup>; Marco Boettger<sup>3</sup>; Vincent Larraillet<sup>3</sup>; <sup>1</sup>*ProteinMetrics LLC, Cupertino, CA*; <sup>2</sup>*Roche Technical Development, Roche Diagnostics GmbH, Penzberg, Germany*; <sup>3</sup>*Roche Innovation Center Munich (RICM), Roche Pharma Research and Early Development (pRED), Penzberg, Germany*
- WP 034 **High Throughput Cysteinylation Screening at mAb Subunit Level Using LC-MS Monitoring Workflow;** Samantha Ippoliti<sup>1</sup>; Bradley Prater<sup>2</sup>; Ying Qing Yu<sup>3</sup>; Mark Wrona<sup>3</sup>; Nick Pittman<sup>4</sup>; Guillaume Bechade<sup>4</sup>; Scott Berger<sup>3</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Similis Bio, Sunnyvale, CA*; <sup>3</sup>*Waters, Milford, MA*; <sup>4</sup>*Waters Corporation, Wilmslow, United Kingdom*

## WEDNESDAY POSTERS

- WP 035 **Complete Characterization of Trastuzumab Deruxtecan, a Cysteine-linked antibody drug conjugate, using high resolution accurate mass (HRAM) Mass Spectrometry;** Xiaoxi Zhang<sup>1</sup>; Min Du<sup>2</sup>; <sup>1</sup>ThermoFisher Scientific, Shanghai, China; <sup>2</sup>Thermo Fisher Scientific, Lexington, MA
- WP 036 **Rapid Quality Assessment of Therapeutic Monoclonal Antibodies through Automated Middle-level Mass Spectrometry;** Andreas Naegeli<sup>1</sup>; Olle De Bruin<sup>2</sup>; Phil Widdowson<sup>1</sup>; Camilla Sivertsson<sup>3</sup>; Gunilla Larsson<sup>2</sup>; Rolf Lood<sup>1</sup>; <sup>1</sup>Genovis AB, Kävlinge, Sweden; <sup>2</sup>Biolnvent International AB, Lund, Sweden; <sup>3</sup>Genovis Inc, Cambridge, MA
- WP 037 **Increased sensitivity and throughput for native intact mass analysis of mAb and ADCs using an online buffer exchange column;** Xiaoxi Zhang<sup>1</sup>; Weijing Liu<sup>2</sup>; Xuepu Li<sup>3</sup>; Min Du<sup>4</sup>; <sup>1</sup>ThermoFisher Scientific, Shanghai, China; <sup>2</sup>ThermoFisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific, Shanghai, China; <sup>4</sup>Thermo Fisher Scientific, Lexington, MA
- WP 038 **The characterization of cysteine conjugated ADCs using native size exclusion chromatography-mass spectrometry (nSEC-MS);** Chendi Niu; AstraZeneca, Gaithersburg
- WP 039 **NIST Biopharmaceutical Reference Materials;** Katharina Yandrofski<sup>1,2</sup>; Ioannis Karageorgos<sup>1,2</sup>; Trina Mouchahoir<sup>1,2</sup>; Zvi Kelman<sup>1,2</sup>; John Schiel<sup>1,2</sup>; John Marino<sup>1,2</sup>; <sup>1</sup>National Institute for Standards and Technology, Gaithersburg, MD; <sup>2</sup>Institute for Bioscience and Biotechnology Research, Rockville, MD
- ARTIFICIAL INTELLIGENCE IN MS INSTRUMENTATION**  
**040-064**
- WP 040 **Machine Learning-Guided Exploration of Known and Unknown Chlorinated Disinfection Byproducts in Nontargeted Mass Spectrometry Analysis;** Tingting Zhao<sup>1</sup>; Nicholas J. P. Wawryk<sup>2</sup>; Shipei Xing<sup>1</sup>; Brian Low<sup>1</sup>; Huaxu Yu<sup>1</sup>; Yukai Wang<sup>1</sup>; Qiming Shen<sup>2</sup>; Xing-Fang Li<sup>2</sup>; Tao Huan<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, BC; <sup>2</sup>University of Alberta, Edmonton, AB
- WP 041 **Versatile artificial intelligence pipeline, designed for diagnosis, prognosis, biomarkers discovery and tissue ImmuneScoring of glioblastoma using SpiderMass technology;** Yanis ZIREM<sup>1</sup>; Léa LEDOUX<sup>1</sup>; Pierre Tirilly<sup>2</sup>; Bertrand Meresse<sup>3</sup>; Claude Alain Maurage<sup>4</sup>; Marie Duhamel<sup>1</sup>; Isabelle Fournier<sup>1</sup>; Michel Salzet<sup>1</sup>; <sup>1</sup>PRISM - Inserm U1192, Villeneuve d'Ascq Cedex France, France; <sup>2</sup>UMR 9189 Cristal, Villeneuve d'Ascq, France; <sup>3</sup>Institute for Translational Research in Inflammation, Villeneuve d'Ascq Cedex France, France; <sup>4</sup>Service de biochimie et biologie moléculaire - CHU de Lille, Lille, France
- WP 042 **Machine Learning-Assisted False Positive Detection in Metabolite Identification Workflows;** Ramon Adàlia<sup>1</sup>; Fabien Fontaine<sup>1</sup>; Luca Moretoni<sup>2</sup>; Ismael Zamora<sup>1</sup>; <sup>1</sup>Mass Analytica, S.L, Sant Cugat del Vallés, Spain; <sup>2</sup>Mass Analytica, S.L, Bettona, Italy
- WP 043 **Towards automated development of charged particle optical instrumentation using a novel optimization framework;** Kilian Huber<sup>1,2</sup>; Tom Wirtz<sup>1</sup>; Quang Hung Hoang<sup>1</sup>; <sup>1</sup>Luxembourg Institute of Science and Technology, Belvaux, Luxembourg; <sup>2</sup>Faculty of Science, Technology and Medicine, University of Luxembourg, Esch-sur-Alzette, Luxembourg
- WP 044 **Characterizing Sampling and Chromatographic Impact on Quantification of Small Molecules in Non-Targeted Analysis;** Jessica Bade<sup>1</sup>; Matthew Turner<sup>1</sup>; Luke Durell<sup>1</sup>; Sean Colby<sup>1</sup>; Sydney Schwartz<sup>1</sup>; Charles Doll<sup>1</sup>; Eva Brayfindley<sup>1</sup>; Fanny Chu<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- WP 045 **DiProQ: A Deep Learning-Driven Method for Differential Analysis in Quantitative Proteomics;** Hojin Yoo<sup>1</sup>; Jose Cruz Castelo<sup>1</sup>; Namgil Lee<sup>1,2</sup>; Heejung Yang<sup>1,3</sup>; <sup>1</sup>Bionsight Inc, Chuncheon-si, South Korea; <sup>2</sup>Department of Information Statistics, Kangwon National University, Chuncheon-si, South Korea; <sup>3</sup>Department of Pharmacy, Kangwon National University, Chuncheon-si, South Korea
- WP 046 **Unsupervised, Masked Pretraining on MS2 Spectra from Peptides for Improving De Novo Sequencing;** Alfred Nilsson<sup>1</sup>; Joel Lapin<sup>2</sup>; Mathias Wilhelm<sup>2</sup>; Lukas Käll<sup>1</sup>; <sup>1</sup>KTH Royal Institute of Technology, Stockholm, Sweden; <sup>2</sup>Technical University of Munich, Freising, Germany
- WP 047 **Revolutionizing Proteomics: Ultra-Fast, High-Accuracy Peptide Sequencing with Enhanced GraphNovo Algorithm;** Zeping Mao<sup>1</sup>; Lei Xin<sup>2</sup>; Shengying Pan<sup>2</sup>; Baozhen Shan<sup>2</sup>; <sup>1</sup>University of Waterloo, Waterloo, ON; <sup>2</sup>Bioinformatics Solutions Inc., Waterloo, ON
- WP 048 **A multidimensional data analysis approach for clinical analysis by mass spectrometry;** Haoyue Zhang<sup>1</sup>; Wenpeng Zhang<sup>1</sup>; Zheng Ouyang<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China
- WP 049 **Tackling mass degeneracy in mass mapping and sequence analysis of nucleic acids;** Daniele Fabris<sup>1</sup>; Daniele Rollo<sup>1</sup>; Thomas Kenderedine<sup>1</sup>; <sup>1</sup>University of Connecticut, Storrs, CT
- WP 050 **Integrating Data Science in MS: Insights into MS/MS Fragmentation and Differential Mass Spectrometry Behaviour;** Stepan Stepanovic<sup>1</sup>; Gerard Hopfgartner<sup>2</sup>; <sup>1</sup>University of Geneva, Olten, Switzerland; <sup>2</sup>University of Geneva, Geneva, Switzerland
- WP 051 **AI Guided Platform for Released Peptide Mapping Method Development Using a Transformer Model;** Mengxiao Liu<sup>1</sup>; Longyun Guo<sup>1</sup>; Bing Ran<sup>1</sup>; Xi Chen<sup>1</sup>; Moyin Zhou<sup>1</sup>; Tongdan Wang<sup>1</sup>; Jincui Huang<sup>1</sup>; <sup>1</sup>WuXi Biologics, Shanghai, China
- WP 052 **[-]SPECFORMER: Pretraining Improves SPECTRUM Embedding through Contrastive Learning with TransFormer;** Tianze Ling<sup>1,2</sup>; Fan Xu<sup>3</sup>; Jun Xia<sup>4</sup>; Stan Z. Li<sup>4</sup>; Yu Wang<sup>3</sup>; Cheng Chang<sup>2</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>National Center for Protein Sciences (Beijing), Beijing, China; <sup>3</sup>Peng Cheng Laboratory, Shenzhen, China; <sup>4</sup>Westlake University, Hangzhou, China
- WP 053 **DeepiRT: Incorporating chromatography information boosts performance of iRT prediction model;** Alexandros Pachos<sup>1</sup>; Sandra Schär<sup>1</sup>; Arthur Viode<sup>1</sup>; An-phi Nguyen<sup>1</sup>; George Rosenberger<sup>1,2</sup>; Oliver M. Bernhardt<sup>1</sup>; Roland Bruderer<sup>1</sup>; Tejas Gandhi<sup>1</sup>; Lukas Reiter<sup>1</sup>; <sup>1</sup>Biognosys AG, Zurich, Switzerland; <sup>2</sup>Bruker Switzerland AG, Faellanden, Switzerland
- WP 054 **Enhancing AlphaFold2 Protein Structure Prediction Using Tandem Mass Spectrometry;** Seonogwang Jeon<sup>1</sup>; Eunok Paek<sup>1</sup>; <sup>1</sup>Hanyang University, Seoul, South Korea
- WP 055 **Machine and Deep Learning Classification of Bacterial Species using Two-Dimensional Tandem Mass Spectrometry;** L. Edwin Gonzalez<sup>1</sup>; Dalton T Snyder<sup>2</sup>; Harman Casey<sup>2</sup>; Yanyang Hu<sup>1</sup>; Joseph V. Caruso<sup>1</sup>; Megan Guetzloff<sup>2</sup>; Nicole Huckaby<sup>2</sup>; Eric T Dziekonski<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, Department of Chemistry, West Lafayette, IN; <sup>2</sup>Teledyne FLIR, West Lafayette, IN
- WP 056 **Artificial Intelligence and Statistics with Mass Spectrometry for Structure Elucidation and Analytical Data Validation of Organic Substances – NPS VeriQon;** Till Orth; Federal Criminal Police Office Germany, Wiesbaden, Germany
- WP 057 **Benchmarking of a machine learning model developed for quantitative metabolomics;** Jeff Pruyne<sup>1</sup>; Joshua D. Lauterbach<sup>1</sup>; Ana S.H. Costa<sup>1</sup>; Devesh Shah<sup>1</sup>; Jack Howland<sup>1</sup>; Luke S Ferro<sup>1</sup>; Timothy Kassis<sup>1</sup>; Mimoun Cadosch Delmar<sup>1</sup>; Jennifer M Campbell<sup>1</sup>; <sup>1</sup>Matterworks, Inc., Somerville, MA
- WP 058 **Towards Science Autonomy for Planetary Missions: Application to Mass Spectrometers for Future Missions to Mars, Titan, and Ocean Worlds;** Victoria Da Poian<sup>1,2</sup>; Eric Lyness<sup>1,2</sup>; Desmond A. Kaplan<sup>1,3</sup>; Ryan M. Danell<sup>1,4</sup>; William B Brinckerhoff<sup>1</sup>; Melissa Trainer<sup>1</sup>; Xiang Li<sup>1</sup>; Andrej Grubisic<sup>1</sup>; Friso H.W. Van Amerom<sup>1</sup>; <sup>1</sup>NASA Goddard Space Flight Center, Greenbelt, MD; <sup>2</sup>Microtel LLC, Greenbelt, MD;



## WEDNESDAY POSTERS

- <sup>3</sup>KapScience LLC, Tewksbury, MA; <sup>4</sup>Danell Consulting, Inc., Winterville, NC
- WP 059 **MS-KGbot: A Conversational AI-Agent for Accessible Mass Spectrometry Metabolomics Data Mining**; Emma Tysinger<sup>1, 2</sup>; Lucas Pradi<sup>2</sup>; Madina Bekbergenova<sup>2, 3</sup>; Benjamin Navet<sup>3</sup>; Olivier Kirchhoffer<sup>4</sup>; Florence Mehl<sup>5</sup>; Marco Pagni<sup>6</sup>; Jean-Luc Wolfender<sup>4</sup>; Fabien Gandon<sup>6</sup>; Louis Felix Nothias<sup>2, 3</sup>; <sup>1</sup>MIT, Cambridge, MA; <sup>2</sup>Université Côte d'Azur, CNRS, ICN, Nice, France; <sup>3</sup>Interdisciplinary Institute for Artificial Intelligence (3iA) Côte d'Azur, Nice, France; <sup>4</sup>School of Pharmaceutical Sciences, University of Geneva, Geneva, Switzerland; <sup>5</sup>Swiss Institute of Bioinformatics (SIB), Lausanne, Switzerland; <sup>6</sup>INRIA, Université Côte d'Azur, CNRS, I3S, Sophia-Antipolis, France
- WP 060 **End-to-end MRM Quantification with Deep Learning Networks**; Mihira Kasun<sup>1</sup>; Pasindu Tennakoon<sup>1</sup>; Rukshan Wijesinghe<sup>1</sup>; Leiver Campeon<sup>1</sup>; Lalin Theverapperuma<sup>1</sup>; Andi Krupke<sup>1</sup>; <sup>1</sup>Expert Intelligence, Santa Clara, CA
- WP 061 **Prediction of 'unspecific' peptide products: enhancing the use of broad-specificity enzymes for mapping of post-translational modifications**; Xuehui Jiang<sup>1</sup>; Victor Spicer<sup>1</sup>; Darien Yeung<sup>1, 2</sup>; Ying Lao<sup>1</sup>; Oleg Krokhin<sup>1, 2, 3</sup>; Rene Peiman Zahedi<sup>1, 2, 3, 4</sup>; <sup>1</sup>Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; <sup>2</sup>Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; <sup>3</sup>Department of Internal Medicine, University of Manitoba, Winnipeg, MB; <sup>4</sup>Paul Albrechtsen Research Institute, Cancer Care Manitoba, Winnipeg, MB
- WP 062 **Nested Machine Learning Pipeline for Precision Targeted Mass Spectrometry**; Jia Fan<sup>1</sup>; Duran Bao<sup>1</sup>; Bo Ning<sup>1</sup>; Tony Hu<sup>1</sup>; <sup>1</sup>Tulane University, New Orleans, LA
- WP 063 **Using Deep Learning for Spectra Translation between Ionization Modalities**; Frederick Zhang<sup>1</sup>; Michael Strobel<sup>2</sup>; Liping Liu<sup>1</sup>; Mingxun Wang<sup>2</sup>; Soha Hassoun<sup>1</sup>; <sup>1</sup>Tufts University, Medford, MA; <sup>2</sup>University of California, Riverside, Riverside, CA
- WP 064 **Super-resolution: what is the best in time with genetic algorithm or in frequency with Artificial Intelligence for Fourier Transform MS?**; Léo CHENEAU<sup>1</sup>; Marc Haegelien<sup>2</sup>; Azad KICHIBAYOV<sup>3</sup>; Anna LEONTEVA<sup>1</sup>; Ulviyya ABDULKARIMOVA<sup>3</sup>; Pierre COLLET<sup>1</sup>; Christian Rolando<sup>2</sup>; <sup>1</sup>Université de Strasbourg, Strasbourg, France; <sup>2</sup>Univ. de Lille, Sciences et Technologies, Villeneuve D'ascq, France; <sup>3</sup>UFAZ - French-Azerbaijani University, Baku, Azerbaijan
- BIOMARKERS: DISCOVERY I**  
**065-101**
- WP 065 **Proteomic analysis of synovial lavage from patients with shoulder instability offers periostin as a molecular indicator for anterior shoulder instability**; Elizabeth Yohannes<sup>1</sup>; Rachel Milam<sup>2</sup>; Brendan Patterson<sup>3</sup>; James V. Nepola<sup>3</sup>; Joseph A. Buckwalter IV<sup>3</sup>; Brian Wolf<sup>3</sup>; Felicity Say<sup>2</sup>; Katherine E. Free<sup>1</sup>; Joseph W. Galvin<sup>2</sup>; <sup>1</sup>Department of Clinical Investigation, Madigan Army Medical Center, Tacoma, WA; <sup>2</sup>Department of Orthopaedic Surgery, Madigan Army Center, Tacoma, WA; <sup>3</sup>Department of Orthopaedic Surgery and Rehabilitation, University of Iowa, Iowa City, IA
- WP 066 **Peptide Biomarkers in Human Breast Milk: Mass Spectrometry-Based In-Solution Proteomics Analysis for Early Detection and Treatment of Breast Cancer Development**; Victor Tochukwu Njoku<sup>1</sup>; Danielle Whitham<sup>1</sup>; Lilian Corrice<sup>1</sup>; Brian T. Pentecost<sup>1, 2</sup>; Kathleen F. Arcaro<sup>2</sup>; Costel C. Darie<sup>1</sup>; <sup>1</sup>Clarkson University, Potsdam, NY; <sup>2</sup>University of Massachusetts Amherst, Amherst, MA
- WP 067 **A comprehensive analysis of serum from women with breast cancer and age-matched controls to determine candidate protein biomarkers**; Danielle Whitham<sup>1</sup>; Pathea S. Bruno<sup>1</sup>; Brian T. Pentecost<sup>1</sup>; Costel C. Darie<sup>1</sup>; <sup>1</sup>Clarkson University, Potsdam, NY
- WP 068 **(H)Ear Me Out: Utilization of Earwax for the Identification of Chemical Markers of Ménière's Disease**; Allix M. Coon<sup>1</sup>; Gavin Setzen<sup>2</sup>; Rabi A. Musah<sup>1</sup>; <sup>1</sup>University at Albany, State University of New York, Albany, NY; <sup>2</sup>Albany ENT & Allergy Services, Albany, NY
- WP 069 **Plasma Metabolomic and Proteomic Profiling of Anxious Dogs by HPLC-MS/MS: A Case-Control Study**; Claudia Gaither<sup>1</sup>; Robert Popp<sup>2</sup>; Francis Beaudry<sup>1</sup>; Christoph H Borchers<sup>3</sup>; Marion Desmarchelier<sup>1</sup>; <sup>1</sup>Université de Montréal Saint-Hyacinthe Campus, Saint-Hyacinthe, QC; <sup>2</sup>MRM Proteomics Inc, Montreal, QC; <sup>3</sup>McGill University, Montreal, QC
- WP 070 **Ultra-deep profiling of human and rodent tissues allows for deepest ever analysis of protein expression levels**; Sandra Schär<sup>1</sup>; Jan Muntel<sup>1</sup>; Marco Tognetti<sup>1</sup>; Christopher Below<sup>1</sup>; Matevsz Stefancic<sup>1</sup>; Igor Sobanski<sup>1</sup>; Roland Bruderer<sup>1</sup>; Lukas Reiter<sup>1</sup>; <sup>1</sup>Biognosys AG, Schlieren, Switzerland
- WP 071 **Proteomics Analysis for Prognosis Biomarkers Clear cell renal carcinoma Patients Undergoing Immunotherapy**; Virginia Campos Silvestrini<sup>1</sup>; Aline Gomes De Souza<sup>1, 2</sup>; Letícia Andrade Costa<sup>1</sup>; Sabrina Baroni<sup>1, 2</sup>; Ana Paula Masson<sup>1</sup>; André Aparecido da Silva Teles<sup>1</sup>; Denise Aparecida Zampieri<sup>3</sup>; Beatriz Boleta Fernandes<sup>3</sup>; José Lopes Bueno Junior<sup>2, 3</sup>; Alexandre Todorovic Fabro<sup>3</sup>; André Schmidt<sup>3</sup>; Fernanda Maria Peria<sup>3</sup>; Fernanda Cristina Gonçalves de Oliveira<sup>3</sup>; Liane Rapatoni<sup>3</sup>; Alison Luis Eburneo Pereira<sup>2</sup>; Olga Laura Sena Almeida<sup>3</sup>; Margaret Castro<sup>3</sup>; Matheus de Aquino Moreira Guimaraes<sup>3</sup>; Rodolfo Borges dos Reis<sup>3</sup>; Valdir Francisco Mugli<sup>3</sup>; Vitor Marcel Faça<sup>1, 2</sup>; Leandro Machado Colli<sup>1, 2, 3</sup>; <sup>1</sup>Medical School of Ribeirão Preto - University of São Paulo, Ribeirão Preto, Brazil; <sup>2</sup>Blood center of Ribeirão Preto, Ribeirão Preto, Brazil; <sup>3</sup>University Hospital of Ribeirão Preto, Ribeirão Preto, Brazil
- WP 072 **Characterization of O-Glycan Profiles of IgA in Ankylosing Spondylitis: A New Approach for Primary and Secondary IgA Nephropathy Differentiation**; Hui-Ling Chiang<sup>1</sup>; Ming-Chi Lu<sup>1, 2</sup>; Ning-Sheng Lai<sup>1</sup>; Chien-Hsueh Tung<sup>1</sup>; Chih-Chia Yu<sup>2</sup>; <sup>1</sup>Division of Immunology, Allergy and Rheumatology, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan; <sup>2</sup>Department of Medical Research, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan
- WP 073 **Pathogenic and Non-pathogenic E. colistrains Discrimination in Urine Samples by LC – IM – MS/MS and Machine Learning**; OROBOLA E. OLAJIDE<sup>1</sup>; Micheal Zirpoli<sup>1</sup>; Jingyi Zheng<sup>1</sup>; Ahmed M. Hamid<sup>1</sup>; <sup>1</sup>Auburn University, AUBURN, AL
- WP 074 **Metabolomics of in vitro skin models: an aging study**; Abigale S Mikolitis<sup>1, 2</sup>; CDT Kye Yu<sup>3</sup>; Ethan M. McBride<sup>1, 2</sup>; Erick S. LeBrun<sup>1, 2</sup>; Zachary J. Sasiene<sup>1, 2</sup>; Mary Donnelly<sup>1, 2</sup>; Emilio S. Rivera<sup>1, 2</sup>; Jennifer Harris<sup>4</sup>; Mohamed Omar Ishak<sup>5</sup>; Emilia A. Solomon<sup>2</sup>; Claire K. Sanders<sup>6, 7</sup>; COL Chi Nguyen<sup>3</sup>; Francisca E. Rodriguez<sup>1, 2</sup>; Trevor G. Glaros<sup>1, 2</sup>; Phillip M. Mach<sup>1, 2</sup>; <sup>1</sup>Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>3</sup>United States Military Academy, West Point, NY; <sup>4</sup>Physical Chemistry and Applied Spectroscopy, Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>5</sup>Transition to Operations/Readiness, Program Project Interface, Los Alamos National Laboratory, Los Alamos, NM; <sup>6</sup>Los Alamos National Laboratory, Los Alamos, NM; <sup>7</sup>Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM
- WP 075 **Discovery of Patient's Specific Biomarker: Concept and Evaluation of a New Diagnosis Strategy**; Bertrand Rochat<sup>1</sup>; Jachen Barblan<sup>2</sup>; <sup>1</sup>Université de Lausanne, Lausanne, Switzerland; <sup>2</sup>Université de Lausanne, Lausanne, Switzerland
- WP 076 **Investigation of idiopathic pulmonary fibrosis pathogenesis by multiple omics approaches**; Fei Wang<sup>1</sup>; Liang Jin<sup>1</sup>; Xue Wang<sup>1</sup>; Baoliang Cui<sup>1</sup>; Jan Schejbal<sup>1</sup>; Erik Hagendorn<sup>1</sup>; Yingli Yang<sup>1</sup>; Lori Duggan<sup>1</sup>; Lucy Phillips<sup>1</sup>; Annette Schwartz<sup>1</sup>; Neha Chaudhary<sup>2</sup>; Sarah Lloyd<sup>3</sup>; Yupeng (David) He<sup>3</sup>; Bhupinder Bawa<sup>3</sup>; Yu Tian<sup>1</sup>; <sup>1</sup>AbbVie Bioresearch Center, Worcester; <sup>2</sup>AbbVie Cambridge

## WEDNESDAY POSTERS

- Research Center, Cambridge, MA; <sup>3</sup>AbbVie Inc., North Chicago, IL
- WP 077 **In-depth Analysis of Plasma Proteomics: Are We Enriching Extracellular Vesicles, Platelets, or Soluble Proteins?**; Chiara Guerrero<sup>1</sup>; Cerina Chhoun<sup>1</sup>; Sara Ceccacci<sup>1</sup>; Ines Metatla<sup>1</sup>; Kevin Roger<sup>1</sup>; <sup>1</sup>Necker Proteomics Platform, INSERM US24, Paris, France
- WP 078 **Bladder Cancer Biomarkers Analysis from Methanol Extracts from Pathology Specimens and Urine using LC-MS/MS**; Alexandra Izydorczak<sup>1</sup>; Wilfrido D. Mojica<sup>1</sup>; Troy D. Wood<sup>1</sup>; <sup>1</sup>SUNY at Buffalo, Buffalo, NY
- WP 079 **Analyzing the Urinary Peptidome to Predict Neurogenic Bladder Risk in Spina Bifida Patients**; Hossein Fazelinia<sup>1</sup>; Hua Ding<sup>1</sup>; Deanne M Taylor<sup>1</sup>; Lynn A Spruce<sup>1</sup>; Jennifer Roof<sup>1</sup>; Dana Weiss<sup>1</sup>; Joanna Fesi<sup>1</sup>; Harry Ischiropoulos<sup>1</sup>; Stephen Zderic<sup>1</sup>; <sup>1</sup>Children's Hospital of Philadelphia, Philadelphia, PA
- WP 080 **Proteomic Characterization of Extracellular Vesicles Purified by Dialysis Membrane Concentration and Electrophoresis as Compared to Standard Ultracentrifugation Techniques**; Nancy Henin<sup>1</sup>; Kenzie Rushing<sup>2</sup>; Katherine Moutis<sup>1</sup>; James N. Higginbotham<sup>3</sup>; Jeffrey L. Franklin<sup>3</sup>; Robert J. Coffey<sup>3</sup>; Amy-Joan L. Ham<sup>1</sup>; <sup>1</sup>Belmont University, College of Pharmacy and Health Sciences, Nashville, TN; <sup>2</sup>Belmont University, College of Science and Math, Nashville, TN; <sup>3</sup>Vanderbilt University Medical Center, Nashville, TN
- WP 081 **Discovery of the serum peptidomic biomarkers related to gestational diabetes mellitus using LC MS/MS coupled with magnetic solid phase extraction**; Xi Gao<sup>1,2</sup>; Guixue Hou<sup>2</sup>; Qunjie Wang<sup>3</sup>; Liang Lin<sup>2</sup>; Jin Zi<sup>2</sup>; Siqi Liu<sup>1,2</sup>; <sup>1</sup>University of Chinese Academy of Sciences, Beijing, China; <sup>2</sup>BGI Genomics, ShenZhen, China; <sup>3</sup>Biosepur, Suzhou, China
- WP 082 **Development of an IP-MALDI Method for Analyzing Endogenous Tau Fragments in Cerebrospinal Fluid**; Kaushi Ohta<sup>1</sup>; Yusaku Hioki<sup>1</sup>; Rie Yamamoto<sup>1</sup>; Masaki Murase<sup>1</sup>; Koichi Tanaka<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Nakagyo-ku, Japan
- WP 083 **HiSorB TD-GC-MS Innovation: Probing Liver Metabolism with Deuterated EVOCs Unveils Potential Novel Enzymatic Pathways and Biomarkers for Disease Diagnosis**; Antonio Murgia<sup>1</sup>; Yusuf Ahmed<sup>1</sup>; Iris Banda<sup>1</sup>; Menisha Manhota<sup>1</sup>; Olga Gandelman<sup>1</sup>; Max Allsworth<sup>1</sup>; Billy Boyle<sup>1</sup>; Daniela Fonseca<sup>1</sup>; Jacob Rudman<sup>1</sup>; Connor Clarke<sup>1</sup>; Alexandra Martin<sup>1</sup>; Giuseppe Ferrandino<sup>1</sup>; <sup>1</sup>Owlstone Medical Ltd, Cambridge, United Kingdom
- WP 084 **An deep plasma workflow applied to discover biomarker candidates of the response to chemo-immunotherapy in patients with thoracic malignancies**; Stefanie Hiltbrunner<sup>1</sup>; Yuehan Feng<sup>2</sup>; Sandra Schaer<sup>2</sup>; Angelica Rigutto<sup>1</sup>; Polina Shichkova<sup>2</sup>; Christopher Below<sup>2</sup>; Luca Raess<sup>2</sup>; Lukas Reiter<sup>2</sup>; Roland Bruderer<sup>2</sup>; Roger Von Moos<sup>3</sup>; Markus Joerger<sup>3</sup>; Alessandra Curioni-Fontecedro<sup>1, 3, 4</sup>; <sup>1</sup>University of Fribourg, Faculty of Science and Medicine, Fribourg, Switzerland; <sup>2</sup>Biognosys AG, Schlieren, Switzerland; <sup>3</sup>Swiss Group for Clinical Cancer Research, Bern, Switzerland; <sup>4</sup>Clinic of Oncology, Cantonal Hospital Fribourg, Fribourg, Switzerland
- WP 085 **Linking local and systemic dysregulations in compromised bone healing under diabetic conditions by proteomics analyses**; Johannes R. Schmidt<sup>1</sup>; Vivien Wiltzsch<sup>1</sup>; Klaudia Adamowicz<sup>2</sup>; Lis Arend<sup>3</sup>; Chit Tong Lio<sup>2</sup>; Daniela Dias<sup>4</sup>; Jörg Lehmann<sup>1</sup>; Thomas Lingner<sup>5</sup>; Olga Tsoy<sup>2</sup>; Patrina S.P. Poh<sup>4</sup>; Tanja Laske<sup>2</sup>; Jan Baumbach<sup>2</sup>; Stefan Kalkhof<sup>1, 6</sup>; <sup>1</sup>Department of Preclinical Development and Validation, Fraunhofer Institute for Cell Therapy and Immunology IZI, Leipzig, Germany; <sup>2</sup>Institute for Computational Systems Biology, University of Hamburg, Hamburg, Germany; <sup>3</sup>Data Science in Systems Biology, Technical University of Munich, Munich, Germany; <sup>4</sup>Julius Wolff Institute, BIH at Charité – Universitätsmedizin Berlin, Berlin, Germany; <sup>5</sup>Genevention GmbH, Göttingen, Germany; <sup>6</sup>Institute for Bioanalysis, Coburg University of Applied Sciences and Arts, Coburg, Germany
- WP 086 **Proteomics Profiling of Mdk Knockout/5x<sup>3</sup>FAD Mice**; Shu Yang<sup>1</sup>; Ya Huang<sup>1</sup>; Zhiping Wu<sup>1</sup>; Yun Jiao<sup>1</sup>; Ping-Chung Chen<sup>1</sup>; Junmin Peng<sup>1</sup>; <sup>1</sup>St Jude Children's Research Hospital, Memphis, TN
- WP 087 **Exploring the Interplay of Brain Tumors and Neurodegenerative Disorders: A Comprehensive Big Data Analysis**; Sanjeeva Srivastava<sup>1</sup>; Deeptarup Biswas<sup>1</sup>; Sanjyot Vinayak Shenoy<sup>1</sup>; Ankit Halder<sup>1</sup>; Aparna Chauhan<sup>1</sup>; Advait Padhye<sup>1</sup>; Yash Choudhary<sup>1</sup>; <sup>1</sup>IIT Bombay, Mumbai, India
- WP 088 **Correlation of metabolomics-derived biomarkers for radiation-induced injury with clinical outcome assessments**; Swarnima Pandey<sup>1</sup>; Nageswara Pilli<sup>1</sup>; William T Andrews<sup>1</sup>; Ludovic Muller<sup>1</sup>; Mehari Weldemariam<sup>1</sup>; Maureen A Kane<sup>2</sup>; <sup>1</sup>University of Maryland, Baltimore, Baltimore, MD; <sup>2</sup>University of Maryland, Baltimore, Baltimore, MD
- WP 089 **Proteogenomic analysis of ovarian cancer reveals a signature to predict platinum refractoriness**; Jeff Whiteaker<sup>1</sup>; Shrabanti Chowdhury<sup>2</sup>; Jacob J Kennedy<sup>1</sup>; Richard Ivey<sup>1</sup>; Marcin Cieslik<sup>3</sup>; Pei Wang<sup>2</sup>; Michael Birrer<sup>1</sup>; Amanda Paulovich<sup>1</sup>; <sup>1</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>2</sup>Icahn School of Medicine at Mount Sinai, New York, NY; <sup>3</sup>University of Michigan School of Medicine, Ann Arbor, MI; <sup>4</sup>University of Arkansas for Medical Sciences, Little Rock, AR
- WP 090 **The Risk of Using Underpowered Proteomic Studies and the Potential of Using Well-powered Cohorts**; Oliver KO Lindhorst<sup>1</sup>; Dylan Nicholas T Tabang<sup>1, 2</sup>; Arthur Viode<sup>1, 2</sup>; Asher Salmon<sup>1</sup>; Lise Nigrovic<sup>1, 2</sup>; Jonathan R Krieger<sup>3</sup>; Judith A Steen<sup>1, 2</sup>; Hanno Steen<sup>1, 2</sup>; <sup>1</sup>Boston Children's Hospital, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>Brucker Ltd., Milton, ON
- WP 091 **Unveiling Potential Endogenous Peptide Biomarkers for Hepatocellular Carcinoma in Serum of Patients with Liver Cirrhosis**; Muhammad Salman Sajid<sup>1</sup>; Habtom Resson<sup>1</sup>; <sup>1</sup>Georgetown University, Washington, DC
- WP 092 **Exploring Novel Low Abundant Medium Size Serum Protein Biomarkers for Hepatocellular Carcinoma in Patients with Liver Cirrhosis**; Muhammad Salman Sajid<sup>1</sup>; Habtom Resson<sup>1</sup>; <sup>1</sup>Georgetown University, Washington, DC
- WP 093 **Dynamic proteomic and phosphoproteomic atlas of neuron maturation with amyloid precursor protein mutation**; Ying Hao<sup>1</sup>; Ziyi Li<sup>1</sup>; Erika Lara Flores<sup>1</sup>; Jasmin Camacho<sup>1</sup>; Benjamin Jin<sup>1</sup>; Lily Cornelius<sup>1</sup>; Sydney Klaisner<sup>1</sup>; Yue A Qi<sup>1</sup>; <sup>1</sup>National Institutes of Health, Bethesda, MD
- WP 094 **N-Glycosylation of IgA in Ankylosing Spondylitis: Unveiling a Specific Inflammatory Biomarker and Exploring its Potential in Macrophage-Driven Innate Immunity**; Hui-Ling Chiang<sup>1</sup>; Ning-Sheng Lia<sup>1</sup>; Chien-Hsueh Tung<sup>1</sup>; Ming-Chi Lu<sup>1, 2</sup>; Yi-Ling Ye<sup>3</sup>; Chih-Chia Yu<sup>2</sup>; <sup>1</sup>Division of Immunology, Allergy and Rheumatology, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan; <sup>2</sup>Department of Medical Research, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan; <sup>3</sup>Department of Biotechnology, National Formosa University, Huwei, Taiwan
- WP 095 **Identification of Non-Angiotensin II ACE Products that Enhance Immunity**; Neethu G Issac<sup>1</sup>; Catalina Avendaño<sup>1</sup>; Daniel Röth<sup>1</sup>; Kenneth E. Bernstein<sup>2</sup>; Markus Kalkum<sup>1</sup>; <sup>1</sup>City of Hope, Beckman Research Institute, Department of Immunology and Theranostics, Duarte, CA; <sup>2</sup>Cedars-Sinai Medical Center, Los Angeles, CA
- WP 096 **Comprehensive workflow for extraction, purification, and accelerated digestion of proteins from Mammalian cells**; Debadeep Bhattacharyya<sup>1</sup>; Patrick McCarthy<sup>2</sup>; Sameer Vasantgadkar<sup>2</sup>; Elisabeth Pundt<sup>2</sup>; Eugenio Daviso<sup>2</sup>; Ulrich Thomann<sup>2</sup>; <sup>1</sup>Covaris, Lexington, MA; <sup>2</sup>Covaris, LLC, Woburn, MA
- WP 097 **High throughput mass spectrometry measure of metabolites and lipids across human populations**; Mo

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- WP 098 **Blood metabolome profiling reveals markers for diabetes-associated kidney disease in Asian Indians;** Jain<sup>1</sup>; Jeramie Watrous<sup>1</sup>; Tao Long<sup>1</sup>; Saumya Tiwari<sup>1</sup>; Tanya Nguyen<sup>1</sup>; Kate Gallagher<sup>1</sup>; <sup>1</sup>*Sapient, San Diego, CA*
- WP 099 **Investigation of the effects of overexpression of Human Jumping Translocation Breakpoint (JTB) Protein using in-solution digestion-based Proteomics;** Taniya Modhishika Jayaweera<sup>1</sup>; Madhuri Jayathirtha<sup>1</sup>; Danielle Whitham<sup>1</sup>; Costel C. Darie<sup>1</sup>; <sup>1</sup>*Biochemistry and Proteomics Laboratories, Department of Chemistry and Biomolecular Science, Clarkson University, Potsdam, NY*
- WP 100 **Evaluation of Extracellular Vesicle Isolation Methods from CSF for high-throughput HD Biomarkers Identification;** Chrisovalantis Papadopoulos<sup>1</sup>; Mari Aaltonen<sup>2</sup>; Olga Shatnyeva<sup>3</sup>; Elena Kunold<sup>2</sup>; Thomas Wild<sup>2</sup>; Carleen M Kluger<sup>2</sup>; Doris Staudt<sup>2</sup>; Christoph Schaab<sup>2</sup>; Denise Hartung<sup>3</sup>; Kristin Schneider<sup>4</sup>; Nora Olszok<sup>4</sup>; Farah Aqel<sup>3</sup>; Jim Rosinski<sup>5</sup>; Jian Chen<sup>5</sup>; Thomas F. Vogt<sup>5</sup>; Ramee Lee<sup>5</sup>; <sup>1</sup>*Evotec SE, Hamburg, Germany*; <sup>2</sup>*Evotec München GmbH, Neuried, Germany*; <sup>3</sup>*Evotec International GmbH, Göttingen, Germany*; <sup>4</sup>*Evotec SE, Göttingen, Germany*; <sup>5</sup>*CHDI Foundation, Princeton, NJ*
- WP 101 **Peptidomic analysis of breast milk and serum from donors with Breast Cancer and matched Controls for biomarker discovery;** Pathea S. Bruno<sup>1</sup>; Danielle Whitham<sup>1</sup>; Isabella Pelkey<sup>1</sup>; Brian T. Pentecost<sup>1,2</sup>; Kathleen F. Arcaro<sup>2</sup>; Costel C. Darie<sup>1</sup>; <sup>1</sup>*Clarkson University, Potsdam, NY*; <sup>2</sup>*University of Massachusetts Amherst, Amherst, MA*
- BIOMARKERS: QUANTITATIVE ANALYSIS II**  
102-127
- WP 102 **Mitochondrial quantitative proteomics unveils hypoxia-induced cardiac impairment concomitant increasing of mitochondrial protein;** Pengcheng Fan<sup>1</sup>; *Pharmaron, Germantown, MD*
- WP 103 **Improved liquid chromatography-tandem mass spectrometry analysis of isomeric urinary mercapturic acid metabolites of crotonaldehyde, methacrolein, and methyl vinyl ketone;** Menglan Chen<sup>1</sup>; Steven Carmella<sup>1</sup>; Yingchun Zhao<sup>1</sup>; Stephen Hecht<sup>1</sup>; <sup>1</sup>*Masonic Cancer Center, UMN, Minneapolis, MN*
- WP 104 **Short and Long-term Stability of tobacco specific Nitrosamines (TSNAs) in human Urine;** Baoyun Xia<sup>1</sup>; Vivian Lee<sup>1</sup>; Alexandria-Helen Rollins<sup>1</sup>; Katie Harbin<sup>1</sup>; John Lee<sup>1</sup>; Justin Lamar Brown<sup>1</sup>; Christina Brosius<sup>1</sup>; Tonya Guillot<sup>1</sup>; Chelsea Walker<sup>1</sup>; Lanqing Wang<sup>1</sup>; <sup>1</sup>*Centers for Disease Control and Prevention, Atlanta, GA*
- WP 105 **Total and Free Malondialdehyde (MDA) Determination by a Novel, High-Throughput LC-MS/MS Method with a Derivation and Liquid-Liquid Extraction;** Emily A Epure<sup>1</sup>; Tian-Sheng Lu<sup>1</sup>; Shuyu Hou<sup>1</sup>; <sup>1</sup>*Medpace, Cincinnati, OH*
- WP 106 **Enhancing BBB Integrity Biomarker Quantitation in Neurovascular Disorder Research through Microflow Solutions;** Dhaval Kumar Patel<sup>1</sup>; Ehsan Nozohouri<sup>1</sup>; Ebru Selen<sup>2</sup>; Rahul Baghla<sup>2</sup>; Ulrich Bickel<sup>1</sup>; <sup>1</sup>*Texas Tech University Health Sciences Center, Amarillo, TX*; <sup>2</sup>*SCIEX, Redwood City, CA*
- WP 107 **A highly sensitive quantification method for trace level of oxytocin in urine using mixed-mode solid phase extraction coupled with LC-MS/MS;** Xing Zhang<sup>1</sup>; Lori Lollis Fralick<sup>1</sup>; Kelly Frances Ethun<sup>1</sup>; <sup>1</sup>*Biomarker Core, Emory National Primate Research Center, Emory University, Atlanta, GA*
- WP 108 **High-resolution mass spectrometry peptide quantitation for biomarker verification using data-independent acquisition;** Remco Van Soest<sup>1</sup>; Patrick Pribil<sup>2</sup>; <sup>1</sup>*SCIEX, Redwood City, CA*; <sup>2</sup>*SCIEX, Concord, ON*
- WP 109 **Achieving Improved Precision and Low Carryover in Parallel Reaction Monitoring Mass Spectrometry through Optimized Chromatographic Strategies with uPAC Neo Column;** Yuan Lin<sup>1</sup>; Jeff Op De Beeck<sup>2</sup>; Paul Jacobs<sup>2</sup>; Shanhua Lin<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Sunnyvale, CA*; <sup>2</sup>*Thermo Fisher Scientific, Ghent, Belgium*
- WP 110 **Maximizing detector utilization – Dual-HPLC-MS for the rapid quantification of metabolites in human blood;** Christian Faist<sup>1</sup>; Thorsten Eierhoff<sup>2</sup>; Heiko Hayen<sup>1</sup>; <sup>1</sup>*University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany*; <sup>2</sup>*University Hospital Muenster, Department of Vascular and Endovascular Surgery, Münster, Germany*
- WP 111 **Stability of Urinary Cotinine and Trans-3'-hydroxycotinine Measurements across 2012-2023;** Patrick Bendik<sup>1</sup>; June Feng<sup>1</sup>; Lanqing Wang<sup>1</sup>; <sup>1</sup>*CDC, Atlanta, GA*
- WP 112 **A sensitive HPLC-MS/MS Method for the Determination of Propylene Glycol in Human Plasma Using Surrogate Standard Approach;** Yizhong Zhang<sup>1</sup>; Wenyan Tang<sup>2</sup>; Brian Hee<sup>3</sup>; Qiang Wang<sup>1</sup>; Changming Yang<sup>2</sup>; Wenzhong Liang<sup>2</sup>; Sakambari Tripathy<sup>1</sup>; Katty Wan<sup>3</sup>; <sup>1</sup>*Pfizer Inc., Groton, CT*; <sup>2</sup>*WuXi AppTec (Shanghai) Co., Ltd, Shanghai, China*; <sup>3</sup>*Pfizer Inc., San Diego, CA*
- WP 113 **Advantages of complementary library construction for the identification and quantification of biomarkers for kidney-related diseases from human plasma;** Jake T Kline<sup>1</sup>; Philip M. Remes<sup>2</sup>; Cristina Jacob<sup>2</sup>; Lilian R Heil<sup>2</sup>; Charles Maxey<sup>2</sup>; Stephanie Samra<sup>2</sup>; Scott M Peterman<sup>2</sup>; Claudia Martins<sup>2</sup>; Lorenzo Gallon<sup>3</sup>; Luca Fornelli<sup>1</sup>; <sup>1</sup>*University of Oklahoma, Norman, OK*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*University of Illinois Chicago, Chicago, IL*
- WP 114 **Analysis of Hemorphin Levels in Sickle Cell Disease using PRM-PASEF and Its Association to Pain;** Yanqi Tan<sup>1</sup>; Eduardo De La Toba<sup>1</sup>; Yavnika Kashyap<sup>2</sup>; Robert Molokie<sup>2,3</sup>; Jim Wang<sup>2</sup>; Jonathan Sweedler<sup>1</sup>; <sup>1</sup>*Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, Illinois*; <sup>2</sup>*Department of Pharmaceutical Sciences, University of Illinois Chicago, Chicago, Illinois*; <sup>3</sup>*Department of Medicine, University of Illinois Chicago, Chicago, Illinois*
- WP 115 **Quantification of the Monoclonal Antibody Pembrolizumab in Human Blood Collected via Volumetric Adsorptive Microsampling (VAMS) Technology and Utilizing LC-MS/MS Detection;** Rama Krishna Reddy Voggu<sup>1</sup>; Eric Thomas<sup>1</sup>; <sup>1</sup>*Labcorp Bioanalytical Services LLC, Indianapolis, IN*
- WP 116 **De Novo Assay Development to Quantify Low Abundant Protein Biomarkers by Immunocapture-LC-MS/MS for Cancer Immunotherapy Development;** Naiyu Zheng<sup>1</sup>; Kristin Taylor<sup>1</sup>; Jennifer Postelnek<sup>1</sup>; Sagar Kawle<sup>1</sup>; Huidong Gu<sup>1</sup>; Tracy Tang<sup>1</sup>; Ming Lei<sup>1</sup>; Sonia Dolfi<sup>1</sup>; Graham Yearwood<sup>1</sup>; Jianing Zeng<sup>1</sup>; <sup>1</sup>*Bristol Myers Squibb, Princeton, NJ*
- WP 117 **Plasma Biomarkers Discovery of Multiple System Atrophy Disease Based on Proteomic Landscape;** Longqin Sun<sup>1</sup>; Jingli Li<sup>1</sup>; Songfeng Wu<sup>1</sup>; Ruibing Li<sup>2</sup>; Yan Zhao<sup>1</sup>; <sup>1</sup>*Beijing Qinglian Biotech Co., Ltd., Beijing, China*; <sup>2</sup>*the First Medical Centre, Chinese PLA General Hospital, Beijing, China*
- WP 118 **Magnetic Beads Based Solid Phase Extraction—Innovative Technology for Automated Sample Preparation;** Qunjie Wang<sup>1</sup>; *Suzhou Agile Bio Electronic Technology Co. LTD., Suzhou, China*
- WP 119 **Development of a blood-based multiplex sensitive LC-MS method for neurodegenerative diseases patient stratification : towards an innovative diagnostic tool;** Florine Leipp<sup>1,2</sup>; Jérôme Vialaret<sup>2</sup>; Aurore Jaffuel<sup>3</sup>; Ann-Christin Niehoff<sup>4</sup>; Sylvain Lehmann<sup>2</sup>; Christophe Hirtz<sup>2</sup>; <sup>1</sup>*Shimadzu France, Noisiel, France*; <sup>2</sup>*LBPC-PPC, Montpellier University, IRMB CHU Montpellier, INM INSERM, Montpellier, France*; <sup>3</sup>*Shimadzu Corporation, Nakagyo-ku, Japan*; <sup>4</sup>*Shimadzu Europa GmbH, Duisburg, Germany*

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- WP 120 **Development and Validation of a Liquid Chromatography Tandem Mass Spectrometry Assay for the Quantification of Dapivirine in Human Hair;** Hideaki Okochi<sup>1</sup>; Alexander Louie<sup>1</sup>; Erica Beckerdite<sup>1</sup>; Karen Kuncze<sup>1</sup>; Edward W. Livant<sup>2</sup>; Leslie Z. Benet<sup>1</sup>; Thesla Palanee-Phillips<sup>3, 4</sup>; Nyaradzo M. Mgodli<sup>5</sup>; Monica Gandhi<sup>1</sup>; <sup>1</sup>University of California-San Francisco, San Francisco, CA; <sup>2</sup>Magee Womens Research Institute, Pittsburgh, PA; <sup>3</sup>University of the Witwatersrand, Johannesburg, South Africa; <sup>4</sup>University of Washington, Seattle, WA; <sup>5</sup>University of Zimbabwe, Harare, Zimbabwe
- WP 121 **To Develop a Quantitative Platform for Post-Traumatic Stress Disorder (PTSD) using Targeted Amino Acids and Metabolites as Molecular Biomarkers;** Shih-Shin Liang; Kaohsiung Medical University, Kaohsiung, Taiwan
- WP 122 **A simple derivatization LC/MS/MS method for the quantitation of plasma short-chain fatty acids;** Anna M. Caldwell<sup>1</sup>; Nur N. Z. Kamarunzaman<sup>1</sup>; Ana Rodriguez-Mateos<sup>1</sup>; John M. Halket<sup>1</sup>; <sup>1</sup>King's College London, London, United Kingdom
- WP 123 **Quantification of Frataxin Proteoforms in Blood of Carriers as Biomarkers of Friedreich's Ataxia Using a Triple Quadrupole Mass Spectrometer;** Teerapat Rojsaijakul<sup>1</sup>; David R. Lynch<sup>1</sup>; Clementina Mesaros<sup>1</sup>; Ian Alexander Blair<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA
- WP 124 **Develop and Validated an Ultra-sensitive LC-MS/MS Method to Simultaneously Quantify Aldosterone and Other 4 Steroids in Human Plasma;** Yuhuan Ji<sup>1</sup>; Chenggang Li<sup>1</sup>; Changjian Zhao<sup>1</sup>; Min Meng<sup>1</sup>; Laixin Wang<sup>1</sup>; <sup>1</sup>Resolian China, Chongqing, China
- WP 125 **Comprehensive profiling of data acquisition strategies to optimize clinically-feasible approaches for monitoring predictive phosphorylation markers;** Amy E. Campbell<sup>1</sup>; Pedro Moreno-Cardoso<sup>1</sup>; Luis Nobre<sup>1</sup>; David N Perkins<sup>1</sup>; Josie A Christopher<sup>1</sup>; Janet Kelsall<sup>1</sup>; Weronika E Borek<sup>1</sup>; Andrew Williamson<sup>1</sup>; Arran D Dokal<sup>1</sup>; <sup>1</sup>Kinomica Ltd, Macclesfield, United Kingdom
- WP 126 **Quantitative Analysis of Amino Acids and Acylcarnitines from Isotope-Impregnated Dried Blood Spots Using Mass Spectrometry;** Wenqian Li<sup>1</sup>; Donald H. Chace<sup>2</sup>; Timothy J. Garrett<sup>1</sup>; <sup>1</sup>University of Florida, GAINESVILLE, FL; <sup>2</sup>Capitainer miQro lab, Warwick, Rhode Island
- WP 127 **Long-term reproducibility of trace-level quantification of seven PAH biomarkers in urine by on-line SPE-HPLC-MS/MS;** Yuesong Wang<sup>1</sup>; Erin N. Pittman<sup>1</sup>; Debra A. Trinidad<sup>1</sup>; Kyle Smith<sup>1</sup>; Antonia M. Calafat<sup>1</sup>; Julianne Cook Botelho<sup>1</sup>; <sup>1</sup>CDC, Atlanta, GA
- CANCER RESEARCH I**  
**128-165**
- WP 128 **High Sensitivity Detection of Deuterium-Labelled Volatile Compound Probes with Orbitrap-MS: from in-vitro Headspace to Breath Biopsy for Lung Cancer;** Alexandra Martin<sup>1</sup>; Rob Smith<sup>1</sup>; Jenifer Mizen<sup>1</sup>; Desirée Otero<sup>1</sup>; Iris Banda<sup>1</sup>; Rory Stallard<sup>1</sup>; Ben Taylor<sup>1</sup>; Connor Clarke<sup>1</sup>; Nidhin Shaju<sup>1</sup>; Mohammad Alkaseem<sup>1</sup>; Karina Joyce<sup>1</sup>; Mariana Ferreira Leal<sup>1</sup>; Agnieszka Smolinska<sup>1,2</sup>; Billy Boyle<sup>1</sup>; Max Allsworth<sup>1</sup>; <sup>1</sup>Owlstone Medical Ltd, Cambridge, United Kingdom; <sup>2</sup>Department of Pharmacology and Toxicology, Maastricht University, Maastricht, Netherlands
- WP 129 **Deciphering Proteome-wide Regulatory Landscape of Ferroptosis in Non-Small Cell Lung Cancer;** Xuan Mo<sup>1</sup>; Carlo P. Ramil<sup>1</sup>; Kerrie Simon<sup>1</sup>; Benjamin Ruprecht<sup>1</sup>; An Chi<sup>1</sup>; <sup>1</sup>Chemical Biology, Merck & Co., Inc., Cambridge, MA
- WP 130 **Acalabrutinib and Potential drug-induced organ toxicity (DIOT): Bioactivation characterized by Mass Spectrometry;** Aishah M Alsibae<sup>1</sup>; Haya I Aljohar<sup>1</sup>; Mohamed W. Attwa<sup>1</sup>; Ali S Abdelhameed<sup>1</sup>; Adnan A Kadi<sup>1</sup>; <sup>1</sup>College of Pharmacy, King Saud University, Riyadh, SA, Riyadh, Saudi Arabia
- WP 131 **Assessing Long-Term Stored Tissues for Multi-Omics Data Quality and Proteogenomics Suitability;** Kyujin Song<sup>1</sup>; Jae-Won Oh<sup>1</sup>; Eunok Paek<sup>2, 3, 4</sup>; Joon-Yong An<sup>5, 6, 7</sup>; Se Jin Jang<sup>8</sup>; Min-Sik Kim<sup>9, 10, 11</sup>; Kwang Pyo Kim<sup>1, 12</sup>; <sup>1</sup>Kyung-Hee University, Yong-in, South Korea; <sup>2</sup>Department of Computer Science, Hanyang University, Seoul, South Korea; <sup>3</sup>Institute for Artificial Intelligence Research, Hanyang University, Seoul, South Korea; <sup>4</sup>Department of Artificial Intelligence, Hanyang University, Seoul, South Korea; <sup>5</sup>Department of Integrated Biomedical and Life Science, Korea University, Seoul, South Korea; <sup>6</sup>BK21FOUR R&E Center for Learning Health Systems, Korea University, Seoul, South Korea; <sup>7</sup>School of Biosystem and Biomedical Science, College of Health Science, Korea University, Seoul, South Korea; <sup>8</sup>University of Ulsan College of Medicine, Asan Medical Center, Seoul, South Korea; <sup>9</sup>Department of New Biology, Daegu Gyeongbuk Institute of Science and Technology, Daegu, South Korea; <sup>10</sup>New Biology Research Center, DGIST, Daegu, South Korea; <sup>11</sup>Center for Cell Fate Reprogramming and Control, DGIST, Daegu, South Korea; <sup>12</sup>Kyung Hee Medical Science Research Institute, Seoul, South Korea
- WP 132 **Coupled Proteomic-Bioinformatic Approach to Investigate New Potential Therapeutic Targets for Soft Tissue Sarcoma;** Veronica De Giorgis<sup>1</sup>; Vittoria Federica Borriani<sup>2</sup>; Marcello Manfredi<sup>1</sup>; Virginia Vita Vanella<sup>1</sup>; Elettra Barberis<sup>2</sup>; Maria Rescigno<sup>3</sup>; Luca Tiraboschi<sup>3</sup>; <sup>1</sup>Department of Translational Medicine, University of Piemonte Orientale, Novara, Italy; <sup>2</sup>Department of science technological innovation, University of Piemonte Orientale, Alessandria, Italy; <sup>3</sup>Clinical institute Humanitas IRCCS, Milan, Italy
- WP 133 **Mass spectrometry identifies novel interactors and palmitoylation targets of zDHHC23 in neuroblastoma;** Sally O Oswald<sup>1, 2</sup>; Leonard A Daly<sup>2, 3</sup>; Barry Pizer<sup>3, 4</sup>; Ian A Prior<sup>3</sup>; Violaine See<sup>5</sup>; Claire E Evers<sup>2, 3</sup>; <sup>1</sup>University of Liverpool, Liverpool, United Kingdom; <sup>2</sup>Centre for Proteome Research, Liverpool, United Kingdom; <sup>3</sup>University of Liverpool, Liverpool, United Kingdom; <sup>4</sup>Alder Hey Children's Hospital, Liverpool, United Kingdom; <sup>5</sup>Université de Lyon, Lyon, France
- WP 134 **CETSA MS profile of five breast cancer cell lines correlates with their biological response to clinically used breast cancer medicines;** Tuomas A Tolvanen<sup>1</sup>; Tomas Friman<sup>1</sup>; Merve Kacal<sup>1</sup>; Ying Sun<sup>1</sup>; Laurence Arnold<sup>1</sup>; Daniel Martinez Molina<sup>1</sup>; <sup>1</sup>Pelago Bioscience AB, Solna, Sweden
- WP 135 **Ultra-Deep Proteome of Osteosarcoma Unravels Novel Biomarkers for Drug Targeting;** Joris Maximilian Frenz<sup>1, 2, 3</sup>; Lianghao Mao<sup>2, 3</sup>; Noelle Jung<sup>1, 3</sup>; Dibyendu Seal<sup>1, 3</sup>; Yongjie Wang<sup>1, 3</sup>; Robert Autry<sup>1, 3</sup>; Stefan M. Pfister<sup>1, 3</sup>; Andreas Von Deimling<sup>2</sup>; Andreas E. Kulozik<sup>1, 2, 3</sup>; Ashok Kumar Jayavelu<sup>1, 3</sup>; <sup>1</sup>German Cancer Research Center (DKFZ), Heidelberg, Germany; <sup>2</sup>Heidelberg University Hospital (UKHD), Heidelberg, Germany; <sup>3</sup>Hopp Children's Cancer Center (KITZ), Heidelberg, Germany
- WP 136 **Volatile Analysis of Lung Cancer in a Preclinical Model via Secondary Electrospray Ionization Mass Spectrometry;** Jiangjiang (Chris) Zhu; The Ohio State University, Columbus, OH
- WP 137 **Identifying possible new CAR-T cell immunotherapy targets induced by drug treatment with surface proteomics;** Ruzena Filandrova<sup>1</sup>; Pauline Douglas<sup>1</sup>; Sorana Morrissy<sup>1</sup>; Jennifer Chan<sup>1</sup>; David C Schriemer<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, AB
- WP 138 **Proteomic Analysis of Red Blood Cells Reveals Putative Biomarkers of Prostate Cancer;** Tong Zhang<sup>1</sup>; Zhangyang Xu<sup>2</sup>; Rachel Lawrence<sup>3</sup>; Priscilla Lalli<sup>2</sup>; Yongjie Lu<sup>3</sup>; Tujin Shi<sup>2</sup>; <sup>1</sup>Pacific Northwest National Lab, Richland, WA; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>3</sup>Queen Mary University of London, London, United Kingdom
- WP 139 **Short Gradient NanoLC-DIA-MS-Based Proteomic Profiling of Prostate Cancer Plasma-Derived Extracellular Vesicles Isolated Using Two-Dimensional Size Exclusion Chromatography;** Alan J. Zimmerman<sup>1</sup>; Getulio Pereira De Oliveira Junior<sup>1</sup>; Jacqueline Wood<sup>1</sup>; Alexander R. Ivanov<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA

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- WP 140 **Differential expression of immunogenic cell death modulators in triple negative breast cancer subtypes defined by in situ FFPE sample processing;** Francis Scott Heinemann<sup>1</sup>; Paul Gershon<sup>2</sup>; <sup>1</sup>Hoag Memorial Hospital Presbyterian, Newport Beach, California; <sup>2</sup>UC-Irvine, Irvine, CA
- WP 141 **Quantification of the Anticancer Drug, Busulfan, in Plasma in Less Than 11 Seconds per Sample Using LDTD-MS/MS;** Sylvain Letarte<sup>1</sup>; Mégane Moreau<sup>2</sup>; Serge Auger<sup>2</sup>; Sarah Demers<sup>2</sup>; Jonathan Rochon<sup>2</sup>; Jean Lacoursière<sup>2</sup>; Pierre Picard<sup>2</sup>; <sup>1</sup>Ingenio, Calgary, AB; <sup>2</sup>Phytronix Technologies, Quebec, QC
- WP 142 **Identification and quantification of candidate protein biomarkers in human plasma for early diagnosis of breast cancer;** Margret Thorsteinsdottir<sup>1, 2, 3</sup>; Kristrun Yr Holm<sup>1, 2</sup>; Magnus Gauti Ulfarsson<sup>1, 3</sup>; Valdis Gunnarsdottir Thormar<sup>2, 4</sup>; Finnur Freyr Eiriksson<sup>1, 3</sup>; Yassene Mohammed<sup>5</sup>; Christoph H. Borchers<sup>6, 7, 8, 9</sup>; Sigridur Klara Bodvardsdottir<sup>2, 4</sup>; <sup>1</sup>Faculty of Pharmaceutical Sciences, University of Iceland, Reykjavik, Iceland; <sup>2</sup>BioMedical Center, University of Iceland, Reykjavik, Iceland; <sup>3</sup>ArcticMass, Reykjavik, Iceland; <sup>4</sup>Faculty of Medicine, University of Iceland, Reykjavik, Iceland; <sup>5</sup>Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; <sup>6</sup>Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, McGill University, Montreal, Quebec; <sup>7</sup>Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; <sup>8</sup>Division of Experimental Medicine, McGill University, Montreal, QC; <sup>9</sup>Department of Pathology, McGill University, Montreal, QC
- WP 143 **Developing a multiplexed proteoform reaction monitoring (PFRM) assay for the quantification of intact RAS proteins from cancer cell lines;** Alyssa A Williams<sup>1</sup>; Jake T Kline<sup>1</sup>; Robert A D'Ippolito<sup>2</sup>; Grace M Scheidemantle<sup>2</sup>; Peter H Frank<sup>2</sup>; Dominic Esposito<sup>2</sup>; Caroline J DeHart<sup>2</sup>; Luca Fornelli<sup>1</sup>; <sup>1</sup>University of Oklahoma, Norman, OK; <sup>2</sup>Frederick National Laboratory for Cancer Research, Frederick, MD
- WP 144 **Cardiolipin acyl chain modulation as a therapeutic target in the pediatric brain tumor, embryonal tumor with multilayered rosettes;** Evangelos Liapis<sup>1</sup>; Kelly C O'Neill<sup>1</sup>; Annapurna Pamreddy<sup>1</sup>; Allison Maas<sup>1</sup>; Derek Hanson<sup>1</sup>; Claire Louise Carter<sup>1</sup>; <sup>1</sup>Hackensack Meridian Health, Nutley, NJ
- WP 145 **Molecularly Aware Robotic Surgery with Laser Desorption – Rapid Evaporative Ionisation Mass Spectrometry for Autonomous Surgical Interventions;** Jinshi Zhao<sup>1</sup>; Daniel Simon<sup>1, 2</sup>; Mark Runciman<sup>1</sup>; Haozheng Xu<sup>1</sup>; Amelia Fraser-Dale<sup>1</sup>; Eftychios Manoli<sup>1</sup>; Stamatia Giannarou<sup>1</sup>; George Mylonas<sup>1</sup>; Zoltan Takats<sup>1, 2</sup>; Burak Temelkuran<sup>1, 2</sup>; <sup>1</sup>Imperial College London, London, United Kingdom; <sup>2</sup>Rosalind Franklin Institute, Harwell, United Kingdom
- WP 146 **Assessment of global metabolic changes in antibiotic treated mice and the impact on the pancreatic cancer tumor microenvironment;** Dominik Awad<sup>1</sup>; Li Zhang<sup>1</sup>; Peter Sajjakulnukit<sup>1</sup>; Harrison Wong<sup>1</sup>; Anthony Andren<sup>1</sup>; Damien Sutton<sup>1</sup>; Noah Nelson<sup>1</sup>; Carlos Espinoza<sup>1</sup>; Donnele Daley<sup>1</sup>; Costas A Lyssiotis<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- WP 147 **Extracellular vesicles' lipidome differs between types of cancers as well as between primary and metastatic cancers;** Erika Dorado<sup>1</sup>; James S McKenzie<sup>1</sup>; Stefania Maneta-Stavarakaki<sup>1</sup>; R Charles Coombes<sup>1</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College London, London, United Kingdom
- WP 148 **Studying crosstalk between tumor and microenvironmental cells driving drug response in Acute Myeloid Leukemia using cell-type specific proteomics;** Marija Veličković<sup>1</sup>; Hsin-Yun Lin<sup>2</sup>; Belinda B Garana<sup>1</sup>; Marina A Gritsenko<sup>1</sup>; Reta Birhanu Kitata<sup>1</sup>; Thomas L. Fillmore<sup>1</sup>; Karl K. Weitz<sup>1</sup>; Jeffrey J. Tyner<sup>2</sup>; Sara J.C. Gosline<sup>1</sup>; Anupriya Agarwal<sup>2</sup>; Paul D. Plehowski<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Oregon Health and Science University, Portland, OR
- WP 149 **Protein biomarker discovery across stages of pancreatic neoplasms using mass-spectrometry based proteomics of pancreatic cyst fluid;** Gina Chang<sup>1</sup>; Whitney Smith-Kinnaman<sup>1</sup>; Amber L Mosley<sup>1</sup>; <sup>1</sup>Indiana University School of Medicine, Indianapolis, IN
- WP 150 **Thermal Proteome Profiling to discover novel protein targets of PARP inhibitors;** Li Wang<sup>1</sup>; Jidong Wang<sup>2</sup>; Xiangyi Kong<sup>2</sup>; MD Kamrul Hasan Khan<sup>2</sup>; Xinyan Wu<sup>2</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN; <sup>2</sup>Mayo Clinic, Rochester, MN
- WP 151 **Mass spectrometry-based bulk and single-cell proteomic profiling of CB-5083 resistant colon cancer cells;** Marion Pang<sup>1</sup>; Ting-Yu Wang<sup>1</sup>; Feng Wang<sup>1</sup>; Shan Li<sup>1</sup>; Chai Foong Lai<sup>1</sup>; Baiyi Quan<sup>1</sup>; Yanping Qiu<sup>1</sup>; Tsui-Fen Chou<sup>1</sup>; <sup>1</sup>California Institute of Technology, Pasadena, CA
- WP 152 **Comparison of Mass Spectrometry-Based Proteomics Data from Primary Human and Patient-Derived Xenograft Mouse Tumors;** Fernando Garcia-Marques<sup>1, 2</sup>; Abel Bermudez<sup>1, 2</sup>; Dalin Zhang<sup>3</sup>; Hongjuan Zhao<sup>3</sup>; James D. Brooks<sup>3</sup>; Sharon J Pitteri<sup>1, 4</sup>; <sup>1</sup>Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; <sup>2</sup>Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; <sup>3</sup>Department of Urology, Stanford University School of Medicine, Stanford, CA 94305, Palo Alto, CA; <sup>4</sup>Department of Radiology, Stanford University School of Medicine, Palo Alto, CA, United States, Palo Alto, CA
- WP 153 **Recurrence In Hepatocarcinoma Investigated With Picosecond Infrared Laser Mass Spectrometry: Towards A Rapid Screening Tool For Successful Transplant;** Francis O Talbot<sup>1</sup>; Lan Anna Ye<sup>1</sup>; Michael Woolman<sup>1</sup>; Arash Zarrine-Afsar<sup>2</sup>; Elisa Pasini<sup>1</sup>; Xun Zhao<sup>1</sup>; Jeffery To<sup>1</sup>; Mamatha Bhat<sup>1</sup>; <sup>1</sup>University Health Network, Toronto, ON; <sup>2</sup>Princess Margaret Cancer Centre, University Health Network, Toronto, ON
- WP 154 **Deciphering Medulloblastoma Heterogeneity in the Indian Subpopulation: An FFPE-Based Proteomic Study;** Medha Gayathri J Pai<sup>1</sup>; Avinash Singh<sup>1</sup>; Shilpa Rao<sup>2</sup>; Anita Mahadevan<sup>2</sup>; Sanjeeva Srivastava<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Bombay, Mumbai, India; <sup>2</sup>National Institute of Mental Health and Neurological Sciences, Bengaluru, India
- WP 155 **Discovery and validation of secretory markers-derived from sphingolipid metabolism in Oral Squamous Cell Carcinoma patients through discovery and targeted proteomics;** Avinash Singh<sup>1</sup>; Suraj T<sup>1</sup>; Abhinav Verma<sup>2</sup>; Richa Vaish<sup>3</sup>; Sudhir Nair<sup>4</sup>; Sanjeeva Srivastava<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Bombay, Mumbai, India; <sup>2</sup>Indian Institute of Science Education and Research, Berhampur, India; <sup>3</sup>Tata Memorial Hospital, Mumbai, India; <sup>4</sup>Advance Centre for Treatment Research & Education in Cancer, Mumbai, India
- WP 156 **Multi-Omics Approach based Drug Discovery: Unleashing targets pertaining to Meningioma aggressiveness and evaluating the drug efficacy;** Ankit Halder<sup>1</sup>; Deeptarup Biswas<sup>1</sup>; Archisman Maitra<sup>1</sup>; Sanjeeva Srivastava<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Bombay, Mumbai, India
- WP 157 **Mass spectrometry-based characterization of oxidative damage for different dose rate regimes as a new platform for investigating the FLASH effect;** Sayan Gupta<sup>1</sup>; Jamie Inman<sup>1</sup>; Jared De Chant<sup>1</sup>; Lieselotte Obst-Huebl<sup>1</sup>; Kei Nakamura<sup>1</sup>; Shawn Costello<sup>2</sup>; Darren Kahan<sup>3</sup>; Susan Marqusee<sup>3</sup>; Jian-Hua Mao<sup>1</sup>; Louis Kunz<sup>4</sup>; Marie-Catherine Vozenin<sup>5</sup>; Antoine Snijders<sup>1</sup>; Corie Y Ralston<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, CA; <sup>2</sup>Stanford University, Stanford, CA; <sup>3</sup>University of California, Berkeley, Berkeley, CA; <sup>4</sup>Hôpitaux Universitaires de Genève, Geneva, Switzerland; <sup>5</sup>Hôpitaux Universitaires, Geneva, Switzerland
- WP 158 **Characterization of the Cell-Membrane Proteome as the Interface Between Cancer Cells and the Tumor Microenvironment;** Iulia M. Lazar<sup>1</sup>; Yunqian Zhang<sup>1</sup>; Pratiatha Sarkar<sup>1</sup>; Joshua RS Haueis<sup>1</sup>; Shreya Ahuja<sup>1</sup>; Arba Karcini<sup>1</sup>; <sup>1</sup>Virginia Tech, Blacksburg, Virginia

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- WP 159 **Proteomic Insights of FAK Dependency in Breast Cancer**; Lai Chai Foong<sup>1</sup>; Hope Hua<sup>1</sup>; Wenxuan Huang<sup>1</sup>; Chia Yen Liew<sup>2</sup>; Diana Huynh<sup>1</sup>; Ting-Yu Wang<sup>2</sup>; Baiyi Quan<sup>2</sup>; Yanping Qiu<sup>2</sup>; Timothy Marlowe<sup>3</sup>; Gordon Stott<sup>4</sup>; Andrew Flint<sup>4</sup>; Barbara Mroczkowski<sup>5</sup>; Tsui-Fen Chou<sup>1,2</sup>; <sup>1</sup>*Division of Biology and Biological Engineering, California Institute of Technology, Pasadena, CA*; <sup>2</sup>*Proteome Exploration Laboratory, Beckman Institute, California Institute of Technology, Pasadena, CA*; <sup>3</sup>*The University of Arizona Cancer Center, Phoenix, AZ*; <sup>4</sup>*Leidos Biomedical Research, Inc., Frederick National Laboratory for Cancer Research, National Cancer Institute, Bethesda, MD*; <sup>5</sup>*Division of Cancer Diagnosis and Treatment and Center for Cancer Research, NCI, NIH, Bethesda, MD*
- WP 160 **Comprehensive proteogenomic investigation of high-grade gliomas towards identifying markers of therapeutic potential and drug repurposing for drug candidates**; Ayushi Verma<sup>1</sup>; Prashant Kumar<sup>2</sup>; Sanjeeva Srivastava<sup>3</sup>; <sup>1</sup>*Indian Institute of Technology Bombay, Mumbai, India*; <sup>2</sup>*Karkinos Lab, Mumbai, India*; <sup>3</sup>*Indian Institute of Technology Bombay, Mumbai, India*
- WP 161 **Extracellular Vesicle Proteomics of Primary Human Monocyte-Derived Myeloid Cells**; Carlo Ramil<sup>1</sup>; Handan Xiang<sup>1</sup>; Lisia Cabral<sup>1</sup>; Zhizhang Yin<sup>1</sup>; An Chi<sup>1</sup>; <sup>1</sup>*Merck & Co., Inc., Cambridge, MA*
- WP 162 **Determination of Cellular Kinact/KI for a KRAS inhibitor by LCMS**; Xuele Song; *Merck, Boston, MA*
- WP 163 **Metabolomic analysis of efficiently recovered small extracellular vesicles derived from cancer cells**; Ryosuke Hayasaka<sup>1</sup>; Tomoyoshi Soga<sup>1</sup>; Akiyoshi Hirayama<sup>1</sup>; <sup>1</sup>*Keio University, Tsuruoka, Japan*
- WP 164 **Mechanistic insights into the antitumoral potential of a new silver/selenium based nanosystem revealed by mass spectrometry**; Jose L Luque-Garcia<sup>1</sup>; Pilar Buenadia-Nacarino<sup>1</sup>; Roberto Alvarez-Fernandez Garcia<sup>1</sup>; Blanca Gonzalez<sup>1</sup>; <sup>1</sup>*Complutense University of Madrid, Madrid, Spain*
- WP 165 **A mass spectrometry-based multi-omic approach for the evaluation of rhodium nanoparticles as novel photosensitizers in photodynamic therapy for cancer**; Gabriel A. Peñalver<sup>1</sup>; Andres Machuca<sup>1</sup>; Alejandro Garcia-Garcia<sup>1</sup>; Estefania Garcia-Calvo<sup>1</sup>; Jose L Luque-Garcia<sup>1</sup>; <sup>1</sup>*Complutense University of Madrid, Madrid, Spain*
- CLINICAL ANALYSIS I**  
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- WP 166 **Analysis of influencing factors on venetoclax blood concentration in leukemia patients**; Wenli Sun; *Hebei Yanda Lu Daopei Hospital, Langfang Hebei, China*
- WP 167 **The Clinical Application of Monitoring of Voriconazole and Its Metabolites in Allogeneic Hematopoietic Stem Cell Transplantation Patients**; Wang hong Chun<sup>1</sup>; Wang Lei<sup>2</sup>; <sup>1</sup>*Beijing Lu Daopei Hospital, 22 Tongji Nan Road, Tongzhou District, Beijing, China*; <sup>2</sup>*Hebei Yanda Lu Daopei Hospital, Langfang, China*
- WP 168 **Simultaneous Analysis of Ultrashort-Chain to Long-Chain (C1 to C10) and Alternative Per- and Polyfluorinated Substances in Human Plasma and Serum**; Shun-Hsin Liang<sup>1</sup>; Justin Steimling<sup>2</sup>; <sup>1</sup>*Restek Inc., Bellefonte, PA*; <sup>2</sup>*Restek Corporation, Bellefonte, PA*
- WP 169 **Untargeted Paper Spray Mass Spectrometry (PS-MS): Rapid Diagnosis of Albuminuria Enabling Early Detection and Progression Monitoring of Chronic Kidney Disease**; Igor Pereira<sup>1</sup>; Jindar N.S. Sbotto<sup>1</sup>; Jason L Robinson<sup>2</sup>; Christopher G. Gill<sup>1,3,4,5,6</sup>; <sup>1</sup>*Appl. Env. Res. Labs. (AERL), Nanaimo, BC*; <sup>2</sup>*Health PEI, Charlottetown, PEI*; <sup>3</sup>*Vancouver Island University, Nanaimo, BC*; <sup>4</sup>*University of Victoria, Victoria, BC*; <sup>5</sup>*Simon Fraser University, Burnaby, BC*; <sup>6</sup>*University of Washington, Seattle, WA*
- WP 170 **Biomarkers of parenteral nutrition in newborns and their utility in newborn screening**; Konstantinos Petritis<sup>1</sup>; C. Austin Pickens<sup>1</sup>; Rachel C. Lee<sup>1</sup>; Carla D. Cuthbert<sup>1</sup>; <sup>1</sup>*Centers for Disease Control and Prevention, Atlanta, GA*
- WP 171 **Amplification of collision cross-section differences in metal ions by supramolecular complexation with calixarenes in a Bruker timsTOF instrument**; Liu Yang<sup>1</sup>; Jun J Hu<sup>1</sup>; Fuxing Xu<sup>1</sup>; <sup>1</sup>*Ningbo University, Ningbo, China*
- WP 172 **MONITORING OVULATION BY MEASUREMENT OF PREGNANEDIOL-3-GLUCURONIDE IN SPOT URINE SAMPLES VIA UHPLC-MS/MS**; Laura Leoni<sup>1</sup>; Federico Ponzetto<sup>2</sup>; Federica Rosmini<sup>3</sup>; Mirko Parasiliti Caprino<sup>2</sup>; Fabio Settanni<sup>4</sup>; Antonello Nonnato<sup>4</sup>; Ezio Ghigo<sup>2</sup>; Paolo Moghetti<sup>3</sup>; Giulio Mengozzi<sup>1, 4</sup>; <sup>1</sup>*Clinical Biochemistry Laboratory, Department of Medical Sciences, University of Turin, Turin, Italy*; <sup>2</sup>*Endocrinology, Diabetology and Metabolism, Department of Medical Sciences, University of Turin, Turin, Italy*; <sup>3</sup>*Endocrinology, Diabetes and Metabolism, Department of Medicine, University of Verona, Verona, Italy*; <sup>4</sup>*Clinical Biochemistry Laboratory, City of Health and Science University Hospital, Turin, Turin, Italy*
- WP 173 **Improving Lung Cancer Diagnosis: Exploring the Potential of the MassSpec Pen in non-small cell lung cancer Detection and Subtyping**; Yasmin Shanneik<sup>1</sup>; Bryan Burt<sup>2</sup>; Maheshwari Ramineni<sup>1</sup>; Livia S. Eberlin<sup>1</sup>; <sup>1</sup>*Baylor College of Medicine, Houston, TX*; <sup>2</sup>*University of California, Los Angeles, Los Angeles, CA*
- WP 174 **Collection of trace blood using dedicated device and simultaneous analysis of immunosuppressive drugs in whole blood samples**; Takahiro Goda<sup>1</sup>; Yuki Suzuki<sup>2</sup>; Junichi Masuda<sup>2</sup>; Natsuka Kimura<sup>2</sup>; Kenichi Aizawa<sup>3</sup>; <sup>1</sup>*SHIMADZU Corporation, Kawasaki, Japan*; <sup>2</sup>*SHIMADZU Corporation, Kawasaki, Japan*; <sup>3</sup>*Jichi Medical University, Shimotsuke, Japan*
- WP 175 **Validation of a new fully automated assay of Thiamine-PyroPhosphate and Pyridoxal-5-Phosphate in whole blood using LC-MS/MS**; Joep Vuurpijl<sup>1</sup>; Dennis Van Den Heuvel<sup>2</sup>; Chantal Wilbers<sup>1</sup>; Rein Hoedemakers<sup>1</sup>; Tom Stokhof De Jong<sup>2</sup>; <sup>1</sup>*Jeroen Bosch Ziekenhuis, 's-Hertogenbosch, Netherlands*; <sup>2</sup>*Shimadzu Benelux, 's-Hertogenbosch, Netherlands*
- WP 176 **Paper Spray Mass Spectrometry Utilizing On-Paper Enzyme Hydrolysis of Glucuronide Metabolites for Rapid Drug Quantitation in Urine**; Taelor M. Zarkovic<sup>1,2</sup>; Christopher G. Gill<sup>1,2,3,4,5</sup>; <sup>1</sup>*Appl. Env. Res. Labs. (AERL), Nanaimo, BC*; <sup>2</sup>*University of Victoria, Victoria, BC*; <sup>3</sup>*Vancouver Island University, Nanaimo, BC*; <sup>4</sup>*Simon Fraser University, Burnaby, BC*; <sup>5</sup>*University of Washington, Seattle, WA*
- WP 177 **Quantitative GC-MS Analysis of Feces Short-Chain Fatty Acids: Exploring Intestinal Microbiota-Metabolic Disorders Link in Polycystic Ovary Syndrome**; Evgenii Kukaev<sup>1,2</sup>; Alisa Tokareva<sup>1</sup>; Ekaterina Kirillova<sup>1</sup>; Galina Chernukha<sup>1</sup>; Natalia Starodubtseva<sup>1,3</sup>; Vladimir Frankevich<sup>1</sup>; <sup>1</sup>*National Medical Research Center for Obstetrics Gynecology and Perinatology, Moscow, Russia*; <sup>2</sup>*Talrose Institute for Energy Problems of Chemical Physics, Moscow, Russia*; <sup>3</sup>*Moscow institute of physics and technology, Moscow, Russia*
- WP 178 **Therapeutic Drug Monitoring (TDM) of 26 medications and 2 metabolites in hypertensive patients' urine samples using LC-MS/MS for medication adherence**; Yi Ting Tan<sup>1</sup>; DARYL HEE<sup>1</sup>; <sup>1</sup>*Changi General Hospital, Singapore, Singapore*
- WP 179 **DIAGNOSTIC SCREENING OF COVID-19 BASED ON MULTIOMICS DATA BY HIGH-RESOLUTION MASS SPECTROMETRY (MALDI(+)-TOF MS and ESI(±)-Orbitrap MS)**; Camila Medeiros De Almeida<sup>1</sup>; Larissa Campos Motta<sup>1</sup>; Gabriely Silveira Follis<sup>1</sup>; Kellianny da Penha Barcelos Carvalho<sup>2</sup>; Ricardo Alves Bernardo<sup>3</sup>; Almir Custódio Batista Junior<sup>4</sup>; Andréa Rodrigues Chaves<sup>4</sup>; José Brango-Vanegas<sup>5,6</sup>; Rosiane Andrade Da Costa<sup>5</sup>; Octávio Luiz Franco<sup>5,6</sup>; Frederico Garcia Pinto<sup>7</sup>; Denise Coutinho Endringer<sup>8</sup>; Valério Garrone Barauna<sup>9</sup>; Paulo Roberto Filgueiras<sup>10</sup>; José Geraldo Mill<sup>9</sup>; Wanderson Romão<sup>1,11</sup>; <sup>1</sup>*Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espírito*

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- Santo, Vitória, Brazil; <sup>2</sup>Multivix College Serra, Serra, Brazil; <sup>3</sup>Federal University of Paraná, Curitiba, Brazil; <sup>4</sup>Federal University of Goiás, Goiania, Brazil; <sup>5</sup>Catholic University of Brasília, Brasília, Brazil; <sup>6</sup>Dom Bosco Catholic University, Campo Grande, Brazil; <sup>7</sup>Federal University of Viçosa, Rio Paranaíba, Brazil; <sup>8</sup>Universidade Vila Velha, Vila Velha, Brazil; <sup>9</sup>Department of Physiological Sciences, Federal University of Espírito Santo, Vitória, Brazil; <sup>10</sup>Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil; <sup>11</sup>Federal Institute of Espírito Santo, Brazil, Vitoria, Brazil
- WP 180 **Exploratory Analysis MALDI-TOF MS for Detection of Potential Biomarkers of Acute Kidney Injury in Biofluids from Patients Undergoing Liver Transplantation;** Larissa Campos Motta<sup>1</sup>; Camila Medeiros De Almeida<sup>1</sup>; Gabriely Silveira Folli<sup>1</sup>; José Brango-Vanegas<sup>2</sup>; Rosiane Andrade Da Costa<sup>3</sup>; Octavio Luiz Franco<sup>3, 4</sup>; Paulo Roberto Figueiras<sup>5</sup>; Paula Frizera Vassalo<sup>6</sup>; Vandack Alencar Nobre Júnior<sup>6</sup>; Valério Garrone Barauna<sup>7</sup>; Wanderson Romao<sup>1, 8</sup>; <sup>1</sup>Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil; <sup>2</sup>Catholic University of Brasília, Brasília, Brazil; <sup>3</sup>Catholic University of Brasília, Brasília, Brazil; <sup>4</sup>Dom Bosco Catholic University, Campo Grande, Brazil; <sup>5</sup>Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil; <sup>6</sup>Federal University of Minas Gerais, Hospital das Clínicas of UFMG., Belo Horizonte, Brazil; <sup>7</sup>Department of Physiological Sciences, Federal University of Espírito Santo, Vitória, Vila Velha, Brazil
- WP 181 **Inflammatory signature associated with continuous subcutaneous insulin infusion sites (CSII) in Type1 Diabetes: A Proteomic biomarker study from CSII Cannula;** Katarzyna Dabrowska<sup>1</sup>; John Blanchard<sup>2</sup>; Maya Willey<sup>2</sup>; Krystine Garcia-Mansfield<sup>2</sup>; Ritin Sharma<sup>2</sup>; Bithika Thompson<sup>3</sup>; Patrick Pirrotte<sup>2</sup>; Sampath Rangasamy<sup>2</sup>; <sup>1</sup>City of Hope, Duarte, CA; <sup>2</sup>Translational Genomics Research Institute, Phoenix, AZ; <sup>3</sup>Mayo Clinic, Scottsdale, AZ
- WP 182 **Long-term stability and reproducibility of a nanoparticle-based platform for clinical proteomics of human biofluids;** Carleen M Kluger<sup>1</sup>; Frank Rolfs<sup>1</sup>; Till Kindel<sup>1</sup>; Oliver Kardell<sup>1</sup>; Christian Schiffmann<sup>2</sup>; Barbara Kracher<sup>1</sup>; Andreas Tebbe<sup>1</sup>; <sup>1</sup>Evotec München GmbH, Neuried, Germany; <sup>2</sup>Evotec International GmbH, Göttingen, Germany
- WP 183 **Paper-Based Immunoassay for Multiplexed Detection of Colorectal Cancer Biomarkers Through Direct Paper Spray Mass Spectrometry;** Girish Muralikrishnan<sup>1</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio
- WP 184 **Comprehensive Sample Preparation Workflow for Deparaffinization, Extraction, Purification, and Accelerated Digestion of Proteins from Formalin-Fixed Paraffin-Embedded Tissue;** Debadeep Bhattacharyya<sup>1</sup>; Patrick McCarthy<sup>2</sup>; Sameer Vasantgadkar<sup>2</sup>; Elisabeth Pundt<sup>2</sup>; Eugenio Daviso<sup>2</sup>; Ulrich Thomann<sup>2</sup>; <sup>1</sup>Covaris, Lexington, MA; <sup>2</sup>Covaris, LLC, Woburn, MA
- WP 185 **Developing Global Access to Mass Spectrometry through Research Capacity Building Programs;** Waheed Adeola Adedeji<sup>1</sup>; Taona Emmah Mudhuli<sup>2</sup>; Faithful Makita Chingombe<sup>3</sup>; Mario Golding<sup>4</sup>; Jill Hochreiter<sup>5</sup>; Raymond Cha<sup>6</sup>; Qing Ma<sup>6</sup>; Robin Dfrancesco<sup>6</sup>; Troy D Wood<sup>6</sup>; Gene D. Morse<sup>5</sup>; <sup>1</sup>University of Ibadan, Ibadan, Nigeria; <sup>2</sup>Midlands State University, Gweru, Zimbabwe; <sup>3</sup>University of Zimbabwe, Harare, Zimbabwe; <sup>4</sup>University of the West Indies, Kingston, Jamaica; <sup>5</sup>University at Buffalo, Buffalo, NY
- WP 186 **Machine learning assisted MALDI mass spectrometry for rapid antimicrobial resistance prediction in clinicals;** Hang Li<sup>1</sup>; Weibo Gao<sup>1</sup>; Jinming Zhang<sup>1</sup>; Shuang Li<sup>1</sup>; Shuailong Zhang<sup>1</sup>; <sup>1</sup>Beijing Institute of Technology, Beijing, China
- WP 187 **Novel Cleanup and Derivatization Method for High-Throughput Dried Blood Spot Measurement of** Hormones; Julian Reed; Molecular Testing Labs, Vancouver, WA
- WP 188 **Quantifying long-term stress levels by analyzing cortisol in hair in 8 seconds;** Sarah Demers<sup>1</sup>; Mélanie Mercœur<sup>2</sup>; Mégane Moreau<sup>1</sup>; Serge Auger<sup>1</sup>; Jonathan Rochon<sup>1</sup>; Pierre Picard<sup>1</sup>; Jean Lacoursière<sup>1</sup>; <sup>1</sup>Phytronix Technologies, Quebec City, QC; <sup>2</sup>Bertin Technologies, Montigny-Le Bretonneux, France
- WP 189 **Near Real-Time Monitoring of Blood Biomarkers with "Rapid Proteomics";** Steven Yannone<sup>1</sup>; Simion Kreimer<sup>2, 3</sup>; <sup>1</sup>CinderBio, Berkeley, CA; <sup>2</sup>Cedars-Sinai, Los Angeles, CA; <sup>3</sup>MilliThomson, Los Angeles, CA
- WP 190 **Exploring Different HPLC Column Chemistries for Optimal Separation of 13 Bile Acids by LC-MS/MS;** Haley Berkland<sup>1</sup>; Katharina Schramm<sup>2</sup>; Tatiana Yuzyuk<sup>2</sup>; Paul Connolly<sup>1</sup>; Justin Steimling<sup>1</sup>; Jared Burkhardt<sup>1</sup>; <sup>1</sup>Restek Corporation, Bellefonte, PA; <sup>2</sup>ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT
- WP 191 **Signal-to-noise is not a useful performance metric in quantitative analysis;** Brian A Rappold<sup>1</sup>; Randall K Julian<sup>2</sup>; <sup>1</sup>LabCorp, Raleigh, NC; <sup>2</sup>Indigo BioAutomation, Carmel, Indiana
- WP 192 **Application of Deuterium Labeling Mass Spectrometry for a Rapid Antimicrobial Resistance Assay of ESKAPEE Pathogens;** Josiah Rensner<sup>1</sup>; Paul Lueth<sup>1</sup>; Bryan Bellaire<sup>1</sup>; Orhan Sahin<sup>1</sup>; Young Jin Lee<sup>1</sup>; <sup>1</sup>Iowa State University, Ames, IA
- WP 193 **Quantitation of endogenous steroids in serum using plasma separation cards and triple quadrupole mass spectrometry;** Vikki Johnson<sup>1</sup>; Nicholas Chestara<sup>2</sup>; Yoshiyuki Okamura<sup>3</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Carlsbad, CA; <sup>2</sup>DPX Technologies, La Jolla, CA; <sup>3</sup>Shimadzu Scientific Instruments, Columbia, MD
- WP 194 **Dual nESI/APCI source for Analysis of Complex Mixtures;** RILEY FERGUSON<sup>1</sup>; Dmytro S Kulyk<sup>1</sup>; Abraham Kwame Badu Tawiah<sup>1</sup>; <sup>1</sup>Ohio State University, Columbus, OH
- WP 195 **Elevating Excellence: Pioneering a Holistic Strategy to Minimize Carryover and Boost Precision in Plasma Proteomic Discoveries;** Dave Quilici<sup>1</sup>; Brett Phinney<sup>2</sup>; Michael Krawitzky<sup>3, 4</sup>; Pierre-Olivier Schmitz<sup>5</sup>; <sup>1</sup>University of Nevada Reno, Reno, NV; <sup>2</sup>University of California Davis, Davis, CA; <sup>3</sup>Bruker Daltonics, San Jose, CA; <sup>4</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>5</sup>Bruker France SAS, Wissembourg, France
- WP 196 **Development And Validation Of New Method To Measure Plasma Aldosterone And Renin Activity Using Liquid Chromatography Tandem Mass Spectrometer (LC-MS/MS);** DARYL HEE<sup>1</sup>; Yi Ting Tan<sup>1</sup>; <sup>1</sup>Changi General Hospital, Singapore, Singapore

### COVALENT LABELING AND CHEMICAL CROSSLINKING

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- WP 197 **Photocrosslinking to Study Changes in Histone Structural Dynamics Upon Post Translational Modifications;** Kymeri E. Davis<sup>1</sup>; Melanie Cheung See Kit<sup>1</sup>; Ian K. Webb<sup>1</sup>; <sup>1</sup>IUPUI, Indianapolis, IN
- WP 198 **Evaluating CID and EAD Fragmentation for Improved Localization of Hydroxyl Radical Protein Footprinting (HRPF) Modifications;** Jiana Duan<sup>1</sup>; Emily Hart<sup>1</sup>; Remco Van Soest<sup>2</sup>; Zoe Zhang<sup>2</sup>; Haichuan Liu<sup>2</sup>; Scot Weinberger<sup>1</sup>; <sup>1</sup>GenNext Technologies, Half Moon Bay, CA; <sup>2</sup>SCIEX, Redwood City, CA
- WP 199 **Data-Independent Acquisition As Tool For Quantitative Cross-linking Mass Spectrometry;** Zdenek Kukacka<sup>1</sup>; Valerie Prochazkova<sup>1</sup>; Petr Novak<sup>1</sup>; <sup>1</sup>Institute of Microbiology CAS, Prague, Czech Republic
- WP 200 **FAST PHOTOCHEMICAL OXIDATION OF NUCLEIC ACIDS COUPLED TO HIGH-RESOLUTION MS ANALYSIS;** Marek Polak<sup>1, 2</sup>; Jiří Černý<sup>3</sup>; Daniel Kavan<sup>2, 4</sup>; Michael Volny<sup>4, 5</sup>; Petr Novak<sup>2, 4</sup>; <sup>1</sup>Faculty of Science, Charles University, Prague, Czech Republic; <sup>2</sup>BioCeV – Institute of Microbiology, The Czech Academy of Sciences, Prague, Czech Republic; <sup>3</sup>BioCev – Institute of Biotechnology, The

## WEDNESDAY POSTERS

- Czech Academy of Sciences, Prague, Czech Republic; <sup>4</sup>Charles University, Prague 2, Czech Republic; <sup>5</sup>University of Chemistry and Technology, Prague, Czech Republic
- WP 201 **Astral vs. Exploris: Comparing the Identification of In-Cell Fast Photochemical Oxidation of Proteins Within HEK-293 Cells and PBMCs;** Jalah Morris<sup>1</sup>; Lisa M. Jones<sup>1</sup>; <sup>1</sup>University of California San Diego, La Jolla, CA
- WP 202 **Optimizing data acquisition and analysis in cross-linking mass spectrometry on the Orbitrap Astral instrument;** Max Ruwolt<sup>1</sup>; Lars Muehlberg<sup>1</sup>; Yi He<sup>2</sup>; Diogo Borges Lima<sup>1</sup>; Rosa Viner<sup>2</sup>; Fan Liu<sup>1, 3</sup>; <sup>1</sup>Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; <sup>2</sup>ThermoFisher Scientific, San Jose, CA; <sup>3</sup>Charité, Universitätsmedizin Berlin, Berlin, Germany
- WP 203 **Probing epichaperome structure in mouse embryonic stem cells using native gel electrophoresis and a novel high-throughput in-gel crosslinking method;** Luke A Botticelli<sup>1</sup>; Seth McNutt<sup>1</sup>; Feixia Chu<sup>1</sup>; <sup>1</sup>University of New Hampshire, Durham, NH
- WP 204 **Characterization of Antibody Binding Epitopes Using Carbene Chemical Footprinting and Electron Activated Dissociation;** Fan Zhang<sup>1</sup>; Haichuan Liu<sup>2</sup>; Benjamin Bell<sup>1</sup>; Remco van Soest<sup>2</sup>; Zoe Zhang<sup>2</sup>; Breanna Vollmar<sup>1</sup>; Shree Bhagwat<sup>1</sup>; Laurence Fayadat-Dilman<sup>1</sup>; Elliott Jones<sup>2</sup>; Jason Hogan<sup>1</sup>; <sup>1</sup>Merck, South San Francisco, CA; <sup>2</sup>SCIEX, Redwood City, CA
- WP 205 **Covalent Labeling to Probe a Protein with an Intrinsically Disordered Domain;** Evan N Whitford<sup>1,2</sup>; Philip C. Lacey<sup>1,2</sup>; Elijah Day<sup>1, 2</sup>; Steffen Lindert<sup>1, 2</sup>; Vicki H. Wysocki<sup>1, 2, 3</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; <sup>2</sup>Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH; <sup>3</sup>Campus Chemical Instrumentation Center, The Ohio State University, Columbus, OH
- WP 206 **Fast photochemical oxidation of proteins for understanding proteoform differences implicated in racial health disparities associated with triple negative breast cancer;** Jorge Jacinto<sup>1</sup>; Lisa M. Jones<sup>1</sup>; <sup>1</sup>University of California, San Diego, La Jolla, CA
- WP 207 **Comprehensive proteomic analysis of modulating proteins from calcium sensitive cells in circuits;** Alexandria S. Battison<sup>1</sup>; Jeremy Borniger<sup>1</sup>; Jeremy Balsbaugh<sup>2</sup>; <sup>1</sup>Cold Spring Harbor Laboratory, Cold Spring Harbor, NY; <sup>2</sup>University of Connecticut Proteomics and Metabolomics Facility, Storrs, CT
- WP 208 **Probing the Interactions of IGF2 with the Entire Extracellular Region of CI-MPR using Hydroxyl Radical Protein Footprinting;** Sandeep K. Misra<sup>1</sup>; Richard Bohnsack<sup>2</sup>; Nancy Dahms<sup>2</sup>; Joshua S Sharp<sup>3</sup>; <sup>1</sup>University of Mississippi, Oxford, MS; <sup>2</sup>Medical College of Wisconsin, Milwaukee, WI; <sup>3</sup>UNIVERSITY OF Mississippi, Oxford, MS
- WP 209 **Testing the Flash Oxidation (FOX) Protein Footprinting System for Probing the Dynamics of the SARS-CoV-2 Spike Glycoprotein Receptor Binding Domain;** Kezia M. Jemison<sup>1</sup>; Fiona L. Kearns<sup>1</sup>; Mac Kevin E. Braza<sup>1</sup>; Mia A. Rosenfeld<sup>1</sup>; Surl-Hee Ahn<sup>2</sup>; Rommie E. Amaro<sup>1</sup>; Lisa M. Jones<sup>1</sup>; <sup>1</sup>UC San Diego, La Jolla, CA; <sup>2</sup>UC Davis, Davis, CA
- WP 210  **$\alpha$ -Methylene- $\beta$ -Lactone Scaffold for Proteome-wide Capture of Biogenic Amine-Protein Interactions;** Clodette Punzalan<sup>1</sup>; Robert Jervine V Ortega<sup>1</sup>; Jose Intano Jr. <sup>1</sup>; Amy R Howell<sup>1</sup>; Xudong Yao<sup>1</sup>; <sup>1</sup>University of Connecticut - Storrs, Storrs Mansfield, CT
- WP 211 **Evaluating effective reagents for tyrosine bioconjugation by mass spectrometry;** Sharel Cornelius<sup>1</sup>; Adway Ouseph Zacharias<sup>1</sup>; Saiful M Chowdhury<sup>1</sup>; <sup>1</sup>University of Texas at Arlington, Arlington, TX
- WP 212 **Footprinting MS Elucidates the Binding Site of oligomeric Amyloid Beta with sTREM2;** Wesley J. Wagner<sup>1</sup>; Thomas J. Brett<sup>2</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>Washington University School of Medicine, St. Louis, MO
- WP 213 **Novel mass spec-cleavable protein crosslinking agents for detecting direct residue-residue contacts;** Biorn-Erik Wulff<sup>1</sup>; Joshua E. Elias<sup>2</sup>; Pehr A.B. Harbury<sup>1</sup>; <sup>1</sup>Stanford University, Stanford, CA; <sup>2</sup>Chan Zuckerberg Biohub, San Francisco, CA
- WP 214 **Chemical and UV-mediated protein-DNA/RNA XL-MS used for establishing an inventory of DNA-/RNA-binding proteins in mitochondria;** Henri Göther<sup>1,2</sup>; Monika Raabe<sup>1</sup>; Aleksandar Chernev<sup>1</sup>; Juan Tasis Galarza<sup>1</sup>; Luis D Cruz-Zaragoza<sup>3</sup>; Peter Rehling<sup>3</sup>; Henning Urlaub<sup>1,2</sup>; <sup>1</sup>Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; <sup>2</sup>Bioanalytics Group, Institute of Clinical Chemistry, University Medical Center Göttingen, Göttingen, Germany; <sup>3</sup>Department of Cellular Biochemistry, University Medical Center Göttingen, Göttingen, Germany
- WP 215 **Singlet oxygen may serve as a probe for protein footprinting;** Marek Polak<sup>1</sup>; Lukáš Fojtík<sup>1, 2</sup>; Jasmína Portašiková<sup>1,2</sup>; Daniel Kavan<sup>1,2</sup>; Petr Man<sup>1,2</sup>; Michael Volny<sup>2, 3</sup>; Petr Novak<sup>1, 2</sup>; <sup>1</sup>Institute of Microbiology of the Czech Academy of Sciences, Prague, Czech Republic; <sup>2</sup>Faculty of Science, Charles University, Prague, Czech Republic; <sup>3</sup>Institute of Microbiology of the Czech Academy of Sciences, 142 20, Prague, Czech Republic
- WP 216 **Why are crosslinking yields so low? Insights from click-based protein crosslinking;** Nicholas Brodie<sup>1</sup>; Bruno C Amaral<sup>1</sup>; Andrew RM Michael<sup>1</sup>; David C Schriemer<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, AB
- WP 217 **DSBSO-based XL-MS Analysis of Breast Cancer PDX Tissues to Delineate Protein Interaction Network in Clinical Samples;** Fenglong Jiao<sup>1</sup>; Clinton Yu<sup>1</sup>; Wheat Andrew<sup>1</sup>; Lijun Chen<sup>2</sup>; Tung-Shing Mamie Lih<sup>2</sup>; Hui Zhang<sup>2</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>University of California Irvine, Irvine, CA; <sup>2</sup>Johns Hopkins University, Baltimore, MD
- WP 218 **Application of Methionine Oxidation Footprinting in Intact Proteins (MOFIP) to Mouse Brain;** Anju Teresa Sunny<sup>1</sup>; Kellye Cupp-Sutton<sup>1</sup>; Patrycja Szamweber<sup>1</sup>; Yanting Guo<sup>2</sup>; Laura-Isobel McCall<sup>3</sup>; Si Wu<sup>1</sup>; <sup>1</sup>University of Alabama, Tuscaloosa, AL; <sup>2</sup>University of Oklahoma, Norman, OK; <sup>3</sup>San Diego State University, San Diego, CA
- WP 219 **Triangulating Protein Interactions: Expanding Proteomic Insights with Three-Site Cross-Linking;** Clinton Yu<sup>1</sup>; Xiaorong Wang<sup>1</sup>; Eric Novitsky<sup>1</sup>; Paul Morenkov<sup>1</sup>; Scott Rychnovsky<sup>1</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>University of California, Irvine, Irvine, CA
- WP 220 **Silyl Ether Enables High Coverage Chemoproteomic Interaction Site Mapping;** Chau Ngo; <sup>1</sup>University of California Los Angeles, Los Angeles, CA
- WP 221 **Binding Efficiency Analysis of PEGylated Aptamers by LC-MS;** Cole D. Babcock<sup>1, 2</sup>; Makan Golizeh<sup>1</sup>; <sup>1</sup>Concordia University of Edmonton, Edmonton, AB; <sup>2</sup>Babcocks Synthetics Ltd., Wainwright, AB
- WP 222 **Computational Approach to Understanding Nitrile Imines as Photocrosslinkers in Gas-Phase Peptide Scaffold Ions;** Kim Vu<sup>1</sup>; Hongyi Zhu<sup>1</sup>; František Tureček<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA

### DRUG DISCOVERY: QUALITATIVE AND QUANTITATIVE 223-247

- WP 223 **An exploration of novel electrophiles in the context of a living cell using an Inverse Drug Discovery approach;** Sarah M Norman<sup>1</sup>; Zhen Li<sup>1</sup>; Leonard Yoon<sup>1</sup>; Jin-Quan Yu<sup>1</sup>; Jeff W Kelly<sup>1</sup>; <sup>1</sup>Scipps Research Institute, San Diego
- WP 224 **Rapid Point-of-Care Quantitative Analysis of HIV Medications using Two-Dimensional Tandem Mass Spectrometry (2D MS/MS);** Yanyang Hu<sup>1</sup>; Joseph V. Caruso<sup>1</sup>; Peter L. Anderson<sup>2</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>University of Colorado Denver, Aurora, CO
- WP 225 **Development and Optimization of an LC-MS/MS Quantitation Method for Drug Analysis in Bovine Rumen;** Ludmyla Santos Tavares<sup>1</sup>; Raymond Zielinski<sup>1</sup>; <sup>1</sup>Zoetis Inc., Kalamazoo, MI
- WP 226 **Improvement of mass spectrum output for separation and determination of chiral compounds by 2D LC and UPC2 systems;** Xiaopeng Wu<sup>1</sup>; Xiaoxia Yang<sup>1</sup>; Peiyun An<sup>1</sup>;



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- WP 227 **The timsTOF Ultra enables deep global ubiquitinomics of ultra-low protein input samples for validating degrader drug targets;** Philipp Strohmidel<sup>1</sup>; Martin Steger<sup>2</sup>; Uli Ohmayer<sup>2</sup>; Björn Schwalb<sup>2</sup>; Torsten Mueller<sup>1</sup>; Christian Albers<sup>1</sup>; <sup>1</sup>*Bruker Daltonics GmbH & Co. KG, Bremen, Germany*; <sup>2</sup>*NEOsphere Biotechnologies GmbH, Planegg, Germany*
- WP 228 **Dual polarity, high-resolution Acoustic Ejection Mass Spectrometry for high-throughput library screening in 1536-well plates;** David Calabrese<sup>1</sup>; Nate Hoxie<sup>1</sup>; Zina Itkin<sup>1</sup>; Meghav Verma<sup>1</sup>; John Janiszewski<sup>1</sup>; Jonathan Shrimp<sup>1</sup>; Kelli Wilson<sup>1</sup>; Sam Michael<sup>1</sup>; Matthew D Hall<sup>1</sup>; Lyle Burton<sup>2</sup>; Tom Covey<sup>2</sup>; Chang Liu<sup>2</sup>; <sup>1</sup>*NIH/NCATS, Rockville, Maryland*; <sup>2</sup>*SCIEX, Concord, ON*
- WP 229 **Determination of a Cucurbit[7]uril (CB[7])–PEG Conjugate in Dog Plasma and Rat Plasma by LC-MS/MS;** Qing Chang<sup>1</sup>; Man Yang<sup>1</sup>; Yanfu Ren<sup>1</sup>; Zhiyu Li<sup>2</sup>; Lili Xing<sup>2</sup>; Yi Tao<sup>2</sup>; Liang Shen<sup>2</sup>; <sup>1</sup>*WuXi AppTec, Suzhou, China*; <sup>2</sup>*WuXi AppTec, Shanghai, China*
- WP 230 **A high-throughput screening platform to probe protein/metabolite interactions enables rapid discovery of functional allosteric binding sites for drug discovery;** Joseph Lapointe<sup>1</sup>; Olga Zurita<sup>1</sup>; Trisha Moro<sup>1</sup>; Gordon Murray<sup>1</sup>; Kaitlyn Selmer<sup>1</sup>; Christopher F Bennett<sup>1</sup>; Melissa J Buskes<sup>1</sup>; Anil Padyana<sup>1</sup>; Maria-Jesus Blanco<sup>1</sup>; Shomit Sengupta<sup>1</sup>; Marion Dorsch<sup>1</sup>; Thomas Roddy<sup>1</sup>; <sup>1</sup>*Atavistik Bio, Cambridge, MA*
- WP 231 **Comprehensive Host Cell Protein Analysis and Viral Protein Identification in AAV Samples Using Optimized Wide Window Acquisition Method;** Shihan Huo<sup>1</sup>; Song Nie<sup>1</sup>; Yongzheng Cong<sup>1</sup>; Shunhai Wang<sup>1</sup>; Ning Li<sup>1</sup>; <sup>1</sup>*Regeneron Pharmaceuticals, Inc., Tarrytown, NY*
- WP 232 **Triple Quadrupole Infrared Matrix-Assisted Laser Desorption Electrospray Ionization Mass Spectrometry for Faster Scans;** James Sawicki<sup>1</sup>; Andrew Radosevich<sup>2</sup>; Fan Pu<sup>3</sup>; Charles Maxey<sup>4</sup>; Alexander Buzenski<sup>3</sup>; Timothy Brayman<sup>3</sup>; Chankdika Amarasinghe<sup>4</sup>; Nari Talaty<sup>3</sup>; Omprakash Nacham<sup>3</sup>; John Shanley<sup>3</sup>; David Chang-Yen<sup>3</sup>; Nathaniel Elsen<sup>3</sup>; Eloy R. Wouters<sup>4</sup>; Jon D Williams<sup>3</sup>; <sup>1</sup>*AbbVie, North Chicago, IL*; <sup>2</sup>*AbbVie, Inc., North Chicago, IL*; <sup>3</sup>*AbbVie Inc., North Chicago, IL*; <sup>4</sup>*ThermoFisher Scientific, San Jose, CA*
- WP 233 **Bioanalytical Characterization and Stability Evaluation of Drug Metabolites in Biological Matrices - A Case Study;** Yongliang (Kevin) Zhang<sup>1</sup>; Georgia Cornelius<sup>1</sup>; Kosea Frederick<sup>2</sup>; Petia Shipkova<sup>1</sup>; France Landry<sup>1</sup>; <sup>1</sup>*Bristol Myers Squibb, Lawrenceville, NJ*; <sup>2</sup>*Bristol Myers Squibb, Cambridge, MA*
- WP 234 **Stereoselective Protein-Probe Reactivity of Fluorotriazines: An Inverse Drug Discovery Exploration;** Karina Nugroho<sup>1</sup>; Gabriel M. Kline<sup>1</sup>; Christian M. Cole<sup>1</sup>; Jeffery W. Kelly<sup>1</sup>; <sup>1</sup>*Scripps Research, La Jolla, CA*
- WP 235 **Innovative orthogonal method for Host Cell Protein characterization combining Immuno-affinity enrichment and MS Analysis;** Noelia De Lama<sup>1, 2</sup>; Diego Bertaccini<sup>3</sup>; Christine Carapito<sup>1, 2</sup>; <sup>1</sup>*Laboratoire de Spectrométrie de Masse BioOrganique, IPHC (UMR 7178), CNRS, Strasbourg, France*; <sup>2</sup>*Infrastructure Nationale de Protéomique ProFI – FR2048, Strasbourg, France*; <sup>3</sup>*Global Analytical Development, Merck KGaA, Darmstadt, Germany*
- WP 236 **Micro-scale ubiquitin-remnant peptide enrichment and MS analysis on the timsTOF Ultra for protein degrader target validation;** Martin Steger<sup>1</sup>; Uli Ohmayer<sup>1</sup>; Björn Schwalb<sup>1</sup>; Henrik Daub<sup>1</sup>; <sup>1</sup>*NEOsphere Biotechnologies GmbH, Planegg, Germany*
- WP 237 **Structure and Dynamics of Glutide Therapeutics Analyzed by Native Mass Spectrometry and Ion Mobility;** Syuan-Ting Kuo<sup>1</sup>; Zhenyu Xi<sup>1</sup>; Xin Yan<sup>1</sup>; David H Russell<sup>1</sup>; <sup>1</sup>*Texas A&M, College Station, TX*
- WP 238 **Comparative Analysis of Recalled Metformin Using SIFT-MS and Liquid Chromatography;** Anthony Qualley<sup>1</sup>; Mark J. Perkins<sup>2</sup>; Vaughan S. Langford<sup>3</sup>; Colin J. Hastie<sup>2</sup>; <sup>1</sup>*Syft Technology, Pittsburgh, PA*; <sup>2</sup>*Element Lab Solutions, Cambridge, United Kingdom*; <sup>3</sup>*Syft Technologies, Christchurch, New Zealand*
- WP 239 **Multomics Analysis of the Lipoygenase Inhibitor, Ureloxastat, a New Therapeutic Targeting Ferroptosis ;** Arba Karcini<sup>1</sup>; Jenna R Mattice<sup>1</sup>; Anna C Krieger<sup>1</sup>; Whitney Lobo<sup>1</sup>; Yuting Mao<sup>2</sup>; Jana Narasimhan<sup>2</sup>; Marla Weetall<sup>2</sup>; Angela Minnella<sup>1</sup>; Jeff Trimmer<sup>1</sup>; Joey C Latham<sup>1</sup>; <sup>1</sup>*PTC Therapeutics, Inc., Mountain View, CA*; <sup>2</sup>*PTC Therapeutics, Inc., Bridgewater, NJ*
- WP 240 **A LC–MS/MS method for the evaluation of cystic fibrosis mucus permeability of drug candidates targeting the Aryl Hydrocarbon Receptor;** Lorenzo Sardelli<sup>1</sup>; Enrica Frasca<sup>1</sup>; Olga Valentina Garbero<sup>1</sup>; Alex Affricano<sup>1</sup>; Claudio Medana<sup>1</sup>; Sonja Visentin<sup>1</sup>; <sup>1</sup>*University of Turin, Torino, Italy*
- WP 241 **Evaluating selectivity, mechanism of action, and efficacy of KT-253, a heterobifunctional MDM2 degrader;** Charles Lincoln Howarth<sup>1</sup>; Min Yuan<sup>1</sup>; Christina Kolodzy<sup>1</sup>; Sarah Martinez<sup>1</sup>; Eric Kuhn<sup>1</sup>; Yogesh Chutake<sup>1</sup>; Joyoti Dey<sup>1</sup>; Nancy Dumont<sup>1</sup>; Douglas Shorten<sup>1</sup>; Juliet Williams<sup>1</sup>; Susanne B Breitkopf<sup>1</sup>; Kirti Sharma<sup>1</sup>; <sup>1</sup>*Kymera Therapeutics, Watertown, MA*
- WP 242 **Heterobifunctional Degradator KT-333 Inhibits Tumor Growth by Induction of Selective Ubiquitination of Lysine Residues on the Surface of STAT3;** Dirk M Walther<sup>1</sup>; Yatao Shi<sup>1</sup>; Christopher M Browne<sup>1</sup>; Caroline Daigle<sup>1</sup>; Xue Fei<sup>1</sup>; Kiran Mahasenan<sup>1</sup>; Anand Ramanathan<sup>1</sup>; Sarah Martinez<sup>1</sup>; Susanne B Breitkopf<sup>1</sup>; Eric Kuhn<sup>1</sup>; Joyoti Dey<sup>1</sup>; Kirti Sharma<sup>1</sup>; <sup>1</sup>*Kymera Therapeutics, Watertown, MA*
- WP 243 **Comprehensive characterization of an anti-GLP1R Antibody-tethered ligand (ATL) and its in vivo biotransformation using immunocapture LC-MS and LC-MS/MS;** Marc Cao<sup>1</sup>; Haiting Zhang<sup>2</sup>; <sup>1</sup>*Regeneron, Tarrytown, NY*; <sup>2</sup>*Regeneron Pharmaceuticals, Tarrytown, NY*
- WP 244 **Multiplexed Biomarker Quantitation Using Parallel Reaction Monitoring (PRM) LC-MS/MS Coupled with FAIMS and the Newomics DuoESI Source;** Keely E. Fuller<sup>1</sup>; Yuehe Ding<sup>2</sup>; Phillip Y. Chu<sup>1</sup>; Jianhui Zhu<sup>2</sup>; Mandy Kwong<sup>1</sup>; Daojing Wang<sup>3</sup>; Jonathan L Josephs<sup>1</sup>; John C. Tran<sup>1</sup>; Chengjie Ji<sup>2</sup>; Rachel Liuging Shi<sup>1</sup>; <sup>1</sup>*Genentech Inc, South San Francisco, CA*; <sup>2</sup>*NovaBioAssays, Boston, Massachusetts*; <sup>3</sup>*Newomics Inc., Berkeley, CA*
- WP 245 **Developing Improved Intact Protein LC/MS Workflows for the Analysis and Quantitation of Adeno-Associated Viral Capsids;** Alyssa Nodland<sup>1</sup>; Roxana Eggleston-Rangel<sup>1</sup>; Michael McGinley<sup>1</sup>; <sup>1</sup>*Phenomenex, Torrance, CA*
- WP 246 **Small Fragment Screening Targeting Stromal Cell Death and Cysteine Activity Mapping in Keratoconus Pathology using TMT-MS;** Xinyue Liu<sup>1</sup>; Ka Yang<sup>1</sup>; Joao A. Paulo<sup>1</sup>; Edward L. Huttlin<sup>1</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup>*Harvard Medical School, Boston, MA*
- WP 247 **Multomics analysis post fluorescence-activated cell sorting – a cautionary tale;** Feroza K. Choudhury<sup>1</sup>; Viji Premkumar<sup>1</sup>; Jana Zecha<sup>1</sup>; Jonathan Boyd<sup>1</sup>; Andrew S. Gaynor<sup>2</sup>; Zengli Guo<sup>3</sup>; Tom Martin<sup>4</sup>; Raffaello Cimbro<sup>5</sup>; Erik L. Allman<sup>1</sup>; Sonja Hess<sup>1</sup>; <sup>1</sup>*Dynamic Omics, Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD*; <sup>2</sup>*Oncology Cell Therapy, ICC, Oncology R&D, AstraZeneca, Gaithersburg, MD*; <sup>3</sup>*Biologics Engineering, Cell Therapeutics & Viral Technologies, AstraZeneca, Gaithersburg, MD*; <sup>4</sup>*Biologics Engineering, Oncology TTD, ADC, AstraZeneca, Gaithersburg, MD*; <sup>5</sup>*Dynamic Omics, Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Cambridge, United Kingdom*

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- WP 248 **End-to-end automated workflow for trace analysis of tire-derived 6-PPD quinone in water by online membrane sampling coupled to ESI-MS/MS;** Joseph Monaghan<sup>1, 2</sup>; Angelina Jaeger<sup>1, 2</sup>; Haley Tomlin<sup>3</sup>; Jamieson Atkinson<sup>3</sup>; Chris G Gill<sup>1, 2, 4, 5</sup>; Erik T Krogh<sup>1, 2</sup>; <sup>1</sup>*Vancouver Island*

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- University, Nanaimo, BC; <sup>2</sup>University of Victoria, Victoria, BC; <sup>3</sup>British Columbia Conservation Foundation, Nanaimo, BC; <sup>4</sup>Simon Fraser University, Burnaby, BC; <sup>5</sup>University of Washington, Seattle, WA
- WP 249 **Detection, Quantification, and Isomer Differentiation of Per- and Polyfluoroalkyl substances (PFAS) using MALDI-TOF with Trapped Ion Mobility;** Aidan J Reynolds<sup>1</sup>; Abby M. Smith<sup>1</sup>; Tian Autumn Qiu<sup>1, 2</sup>; <sup>1</sup>Department of Chemistry, Michigan State University, East Lansing, Michigan; <sup>2</sup>MSU Center for PFAS Research, East Lansing, Michigan
- WP 250 **The Physical and Chemical Characterization of Levitated Microparticles using a Linear Quadrupole Coupled to Electrospray Mass Spectrometry;** Stephanie Salas<sup>1</sup>; Ravleen Kaur Kohli<sup>1</sup>; James F. Davies<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- WP 251 **Characterization of solvothermal liquefaction products of polystyrene, styrene-butadiene rubber and scrap tire waste by APPI FT-ICR MS, 13C-NMR and FT-IR;** Mahmoud Negm<sup>1</sup>; Eemeli Eronen<sup>1</sup>; Marko Mäkinen<sup>1</sup>; Janne Jänis<sup>1</sup>; <sup>1</sup>University of Eastern Finland, JOENSUU, Finland
- WP 252 **Advanced Nontargeted High Resolution Mass Spectrometry Techniques for Revealing Missing Disinfection Byproducts;** Nicholas J. P. Wawryk<sup>1</sup>; Tingting Zhao<sup>2</sup>; Qiming Shen<sup>1</sup>; Tao Huan<sup>2</sup>; Xing-Fang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, AB; <sup>2</sup>University of British Columbia, Vancouver, BC
- WP 253 **Advanced Nontarget Characterization of Amine-containing Compounds in Suwannee River Standard Reference Materials;** Qiming Shen<sup>1</sup>; Nicholas J. P. Wawryk<sup>1</sup>; Tingting Zhao<sup>2</sup>; Di Zhang<sup>1</sup>; Kristin Carroll<sup>1</sup>; Tao Huan<sup>2</sup>; Xing-Fang Li<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, AB; <sup>2</sup>University of British Columbia, Vancouver, BC
- WP 254 **Rapid, Direct Screening of Priority Metal Contaminants in Environmental Systems with a Reactive 3D-Printed Cone Spray Ionization Methodology;** Jonathan N. Chilaka<sup>1</sup>; Ebenezer H. Bondzie<sup>1</sup>; Jamie R. Wieland<sup>1</sup>; Christopher Hamaker<sup>1</sup>; Patrick W. Fedick<sup>2</sup>; Christopher Mulligan<sup>1</sup>; <sup>1</sup>Illinois State University, Normal, IL; <sup>2</sup>Naval Air Warfare Center, Weapons Division (NAWCWD), China Lake, CA
- WP 255 **Speciation of Algae genes using Matrix-Assisted Laser Desorption Ionization to Build a Mass Spectra Database;** Cheyenne D Copling<sup>1</sup>; Kevin R Tucker<sup>2</sup>; Joao Nail<sup>2</sup>; Carolyn Butts-Willmsmeyer<sup>2</sup>; <sup>1</sup>Southern Illinois University of Edwardsville, Edwardsville, IL; <sup>2</sup>Southern Illinois University Edwardsville, Edwardsville, IL
- WP 256 **Detailed characterization of urinary arsenic metabolic profiles with simultaneous elemental and molecular mass spectrometry;** Tetiana Davydiuk<sup>1</sup>; Jagdeesh S. Uppal<sup>1</sup>; Xiufen Lu<sup>1</sup>; Ahsan Habib<sup>2</sup>; Brandon L. Pierce<sup>2</sup>; Jennifer A. Graydon<sup>3</sup>; Megan Reichert<sup>3</sup>; X. Chris Le<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, AB; <sup>2</sup>University of Chicago, Chicago, IL; <sup>3</sup>Alberta Health, Health Protection Branch, Edmonton, AB
- WP 257 **Analysis of Volatile Organic Compounds (VOCs) in Water using Headspace-GCMS in Accordance with US EPA Method 8260D;** Elvi Horiyanto<sup>1</sup>; Chun Kiang Chua<sup>1</sup>; Elgin Guo Wei Ting<sup>1</sup>; Cynthia Lahey<sup>1</sup>; <sup>1</sup>Shimadzu AP, Singapore, Singapore
- WP 258 **Probing Anthropogenic Pollution Profiles of Coastal Ecosystems Through Public Non-Targeted Tandem Mass Spectrometry Data;** Jarmo-Charles Julian Kalinski<sup>1, 2</sup>; Abzer Kelminal Pakkiri Mohamed Shah<sup>3</sup>; Shane Farrell<sup>4</sup>; Lisa Schellenberg<sup>5, 6</sup>; Andreas F. Haas<sup>5</sup>; Rosemary A. Dorrington<sup>2</sup>; Daniel Petras<sup>1, 7</sup>; <sup>1</sup>College of Natural and Agricultural Sciences, University of California Riverside, Riverside, CA; <sup>2</sup>Department of Biochemistry and Microbiology, Rhodes University, Makhanda, South Africa; <sup>3</sup>Functional Metabolomics Lab, Cluster of excellence CMFI, University of Tuebingen, Tuebingen, Germany; <sup>4</sup>Bigelow Laboratory for Ocean Sciences, East Boothbay, ME; <sup>5</sup>Department of Marine Microbiology and Biogeochemistry, Royal Netherlands Institute for Sea Research (NIOZ), Texel, Netherlands; <sup>6</sup>Institute for Biodiversity and Ecosystem Dynamics (IBED), University of Amsterdam, Amsterdam, Netherlands; <sup>7</sup>University of Tuebingen, CMFI Cluster of Excellence, Interfaculty Institute of Microbiology and Infection Medicine, Tuebingen, Germany
- WP 259 **LC/MS quantitative aspects of GenX: impact of pH on dimer formation;** Joshua Shipman<sup>1</sup>; Eduard Rogatsky<sup>1</sup>; <sup>1</sup>Mosaic Diagnostics, Overland Park, KS
- WP 260 **Ion mobility mass spectrometry reveals fluorotelomer ethoxylates in indoor dust and industrial wastewater;** Karl Jobst<sup>1</sup>; Katherine L. Steeves<sup>2</sup>; Meera J. Bissram<sup>2</sup>; Sonya Kleywegt<sup>3</sup>; Douglas Stevens<sup>4</sup>; Frank L. Dorman<sup>5</sup>; Andre J. Simpson<sup>6</sup>; Myrna J. Simpson<sup>6</sup>; Lindsay S. Cahill<sup>2</sup>; <sup>1</sup>Memorial University Of Newfoundland, St. John's, NL; <sup>2</sup>Memorial University of Newfoundland, St. John's, NL; <sup>3</sup>Ontario Ministry of the Environment, Conservation and Parks, Toronto, ON; <sup>4</sup>Waters, Milford, MA; <sup>5</sup>Waters Corporation, Milford, MA; <sup>6</sup>University of Toronto, Toronto, ON
- WP 261 **Separation of PFOS From TDCA Using SelectraCore® C18 HPLC Column by LC-MS/MS Following EPA Method 1633 Requirements;** Arielle Cocozza; UCT, Bristol, PA
- WP 262 **Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous Matrices Using EPA Method 533 with Automated Solid Phase Extraction (SPE);** Renee N.G Huang<sup>1</sup>; Thuy Nguyen<sup>1</sup>; Surjit Saini<sup>1</sup>; <sup>1</sup>Valley Water, San Jose, California
- WP 263 **Multiple Tools for Demanding Needs: Trace Detection of Organochlorine Pesticides by Agilent 7000E and 7010C GC/MS/MS;** Erinn M O'Neill<sup>1</sup>; Alexis Willey<sup>1</sup>; Anastasia Andrianova<sup>1</sup>; <sup>1</sup>Agilent Technologies, Wilmington, DE
- WP 264 **Characterizing the chemical composition of ultrafine particles from non-tailpipe emissions using the thermal desorption chemical ionization mass spectrometer;** Madeline Cooke<sup>1</sup>; Adam E. Thomas<sup>1</sup>; Véronique Perraud<sup>1</sup>; Lisa M. Wingen<sup>1</sup>; Paulus S. Bauer<sup>1</sup>; Michelia Dam<sup>1</sup>; Barbara J. Finlayson-Pitts<sup>1</sup>; James N. Smith<sup>1</sup>; <sup>1</sup>University of California, Irvine, Irvine
- WP 265 **Chemical ionization mass spectrometry analysis of low volatility vapors emitted from automotive braking;** Adam E. Thomas<sup>1</sup>; Madeline E. Cooke<sup>1</sup>; Michelia Dam<sup>1</sup>; Véronique Perraud<sup>1</sup>; Lisa M. Wingen<sup>1</sup>; Michael J. Ezell<sup>1</sup>; Paulus S. Bauer<sup>1</sup>; Barbara J. Finlayson-Pitts<sup>1</sup>; James N. Smith<sup>1</sup>; <sup>1</sup>University of California, Irvine, Irvine, CA
- WP 266 **Development of targeted and non-targeted methods for quantitative and qualitative analysis of per- and polyfluoroalkyl substances in biosolids and biochars;** Emir Nazdraic<sup>1</sup>; Arthur E. Lee<sup>1</sup>; Joshua Cullen<sup>2, 3</sup>; Javier Ordonez-Loza<sup>4, 5</sup>; J. Larry Campbell<sup>1, 6, 7</sup>; Kati Bell<sup>8</sup>; Naomi Klinghoffer<sup>4, 5</sup>; Franco Berruti<sup>4, 5</sup>; W. Scott Hopkins<sup>1, 6, 9</sup>; <sup>1</sup>University of Waterloo, Waterloo, ON; <sup>2</sup>University of Western Ontario, London, ON; <sup>3</sup>Institute for Chemicals and Fuels from Alternative Resources, Ilderton, ON; <sup>4</sup>University of Western Ontario, London, Ontario; <sup>5</sup>Institute for Chemicals and Fuels from Alternative Resources, Ilderton, Ontario; <sup>6</sup>Watermine Innovation, Waterloo, ON; <sup>7</sup>Bedrock Scientific Inc, Milton, ON; <sup>8</sup>Brown and Caldwell, Nashville, TN; <sup>9</sup>Centre for Eye and Vision Research, Hong Kong, Hong Kong
- WP 267 **Chemical and structural characterization of organic aerosol emitted from laboratory burning of Boreal and Arctic peat by 21T FT-ICR MS;** Eric Schneider<sup>1, 2</sup>; Christopher P. Rügner<sup>1, 2</sup>; Anika Neumann<sup>1, 2</sup>; Martha L. Chacón-Patiño<sup>3</sup>; Markus Somero<sup>4</sup>; Meri Ruppel<sup>5</sup>; Mika Ihalainen<sup>4</sup>; Kajjar Köster<sup>4</sup>; Olli Sippula<sup>4</sup>; Hendryk Czech<sup>1, 6</sup>; Ralf Zimmermann<sup>1, 6</sup>; <sup>1</sup>Department of Analytical Chemistry, University Rostock, Rostock, Germany; <sup>2</sup>Department Life, Light & Matter, University Rostock, Rostock, Germany; <sup>3</sup>National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; <sup>4</sup>Department of Environmental and Biological Sciences, University of Eastern Finland, Kuopio, Finland; <sup>5</sup>Atmospheric Composition Unit, Finnish Meteorological Institute, Helsinki, Finland; <sup>6</sup>Joint Mass Spectrometry Centre, Cooperation Group "Comprehensive

## WEDNESDAY POSTERS

- Molecular Analytics*" (CMA), Helmholtz Munich, Munich, Germany
- WP 268 **Identification and quantification of atmospherically relevant organic peroxides in secondary organic aerosol**; Markus Kalberer; *University of Basel, Basel, Switzerland*
- WP 269 **Using a Compact Single Quadrupole LC-MS for PFAS Analysis**; Kathleen K Luo<sup>1</sup>; Om K Shrestha<sup>1</sup>; Megan P Davis<sup>1</sup>; Landon A Wiest<sup>1</sup>; Evelyn H Wang<sup>1</sup>; Michelle Zipse<sup>1</sup>; <sup>1</sup>*Shimadzu Scientific Instruments, Columbia, MD*
- WP 270 **LC-MS/MS analysis of comprehensive PFAS including EPA method 1633 list and ultrashort chain PFAA**; Tanya Napolitano; *Shodex, New York, NY*
- WP 271 **Expanding the LC-MS Workflow to Analyze Ultrashort-chain PFAS Analytes in Aqueous Environmental Samples**; Erika P Portero<sup>1</sup>; Ana Ramos<sup>1</sup>; Lam Leung<sup>1</sup>; <sup>1</sup>*The Chemours Company, Newark, DE*
- WP 272 **Probing sub-10nm nanoparticles chemical composition from reactions of methanesulfonic acid with multifunctional amines using thermal desorption chemical ionization mass spectrometry**; Veronique Perraud<sup>1</sup>; Paulus S. Bauer<sup>2</sup>; Patricia M. Morris<sup>1</sup>; Kanuri Roundtree<sup>1</sup>; Cathy Wong<sup>1</sup>; James N. Smith<sup>1</sup>; Barbara J. Finlayson-Pitts<sup>1</sup>; <sup>1</sup>*UC Irvine, Irvine, CA*; <sup>2</sup>*UC Irvine, Irvine*
- WP 273 **Online Membrane Sampling coupled to ESI-MS for rapid quantification of toxic components in Oil Sands Process-Affected Waters**; Dylan Steenis<sup>1, 2</sup>; Joseph Monaghan<sup>1, 2</sup>; Ian Vander Meulen<sup>3, 4</sup>; Josh Baker<sup>5</sup>; John Headley<sup>4</sup>; Chris G Gill<sup>1, 2, 6, 7</sup>; Erik T Krogh<sup>1, 2</sup>; <sup>1</sup>*Vancouver Island University, Nanaimo, BC*; <sup>2</sup>*University of Victoria, Victoria, BC*; <sup>3</sup>*University of Saskatchewan, Saskatoon, SK*; <sup>4</sup>*Environment Canada, Saskatoon, SK*; <sup>5</sup>*Nautilus Environmental, Burnaby, BC*; <sup>6</sup>*Simon Fraser University, Burnaby, BC*; <sup>7</sup>*University of Washington, Seattle, WA*
- WP 274 **Enhancing LC-MS Strategies for the Characterization and Attribution of AFFF Samples with SLIM-Enabled High-Resolution Ion Mobility**; Thomas Lubinsky<sup>1</sup>; Michelle English<sup>1</sup>; Frederick Strathmann<sup>1</sup>; <sup>1</sup>*MOBILion Systems, Chadds Ford, PA*
- WP 275 **Metabolomic analysis of effects of pollutant mixture released from grafted adipose tissues on fatty acid and lipid metabolism of mice**; Sam Li; *National University of Singapore, Singapore, Singapore*
- WP 276 **Quantification of 8 chlorination Disinfectant byproducts (DBPs) from water using liquid-liquid extraction and Gas Chromatography with Mass Spectrometry**; Jessin Mathai<sup>1</sup>; Shailesh Damale<sup>2</sup>; Anant Lohar<sup>2</sup>; <sup>1</sup>*Shimadzu, Dubai, United Arab Emirates*; <sup>2</sup>*Shimadzu Middle East and Africa FZE, Dubai, United Arab Emirates*
- WP 277 **Exploring honey bee exposome using a novel passive sampler together with low- and high-resolution mass spectrometry: the case of Denmark**; María Murcia-Morales<sup>1</sup>; Francisco José Díaz-Galiano<sup>1</sup>; María Del Mar Gómez-Ramos<sup>1</sup>; José Luis Oller-Serrano<sup>1</sup>; Cristian Valderrama Conca<sup>1</sup>; Jozef J. M. Van Der Steen<sup>2</sup>; Flemming Vejsnæs<sup>3</sup>; Amadeo R. Fernández-Alba<sup>1</sup>; <sup>1</sup>*Chemistry and Physics Department, University of Almería, Agrifood Campus of International Excellence (ceiA3), Almería, Spain*; <sup>2</sup>*Alveus AB Consultancy, Oisterwijk, Netherlands*; <sup>3</sup>*Danish Beekeepers Association, Fulbyvej, Sorø, Denmark*
- WP 278 **Non-targeted screening of unknown per- and polyfluoroalkyl substances in cosmetics and human plasma using ion mobility-mass spectrometry**; Chloe Penney<sup>1</sup>; Xiaolei Li<sup>1</sup>; Roshanak Amiri<sup>1</sup>; Atanu Sarkar<sup>1</sup>; Karl Jobst<sup>1</sup>; <sup>1</sup>*Memorial University of Newfoundland, St. John's, NL*
- WP 279 **Developing a method to monitor the estrogen-inducible proteins in fishes from the Great Lakes upon exposure to environmental contaminants**; Krishan S Weraduwaage<sup>1</sup>; Taniya M Jayaweera<sup>1</sup>; Bernard Crimmins<sup>2</sup>; Sujjan Fernando<sup>2</sup>; Thomas M Holsen<sup>2</sup>; Costel C Darie<sup>1</sup>; <sup>1</sup>*Biochemistry and Proteomics Laboratories, Department of Chemistry and Biomolecular Science, Clarkson University, Potsdam, NY*; <sup>2</sup>*Department of Civil and Environmental Engineering, Clarkson University, Potsdam, NY*
- WP 280 **Utilization of Automated Solvent Extraction with a Triple Quadrupole Mass Spectrometer following EPA Method 1633 for PFAS Analysis in Soil**; Landon A Wiest<sup>1</sup>; Om K Shrestha<sup>1</sup>; Benedict Liu<sup>2</sup>; Kathleen K Luo<sup>1</sup>; Megan Davis<sup>1</sup>; Evelyn H Wang<sup>1</sup>; Alicia Stell<sup>2</sup>; Ruth Marfil-Vega<sup>1</sup>; <sup>1</sup>*Shimadzu Scientific Instruments, Columbia, MD*; <sup>2</sup>*CEM Corporation, Matthews, NC*
- WP 281 **A single and straightforward method for VOCs analysis: Water quality analysis**; Ricardo Tamashiro Reis<sup>1</sup>; Ana Caroline Martimiano<sup>1</sup>; Isabela de Oliveira e Silva<sup>1</sup>; Rodrigo Ossamu Saga Kitamura<sup>1</sup>; <sup>1</sup>*Shimadzu do Brasil, Barueri, Brazil*
- WP 282 **Development of a LCMS Methodology to Characterize and Quantitate Fluorinated Compounds in Consumer Product**; Michael Deible<sup>1</sup>; Logan Miller<sup>2</sup>; Rachel Hale<sup>1</sup>; William Lipps<sup>2</sup>; <sup>1</sup>*RJ Lee Group, Pittsburgh, Pennsylvania*; <sup>2</sup>*Shimadzu Scientific Instruments, Columbia, MD*
- WP 283 **Reversed Phase Separation Improvements for Short Chain PFAS**; Conner McHale<sup>1</sup>; Barry Boyes<sup>1</sup>; Charles Powley<sup>2</sup>; <sup>1</sup>*Advanced Materials Technology, Wilmington, DE*; <sup>2</sup>*Center for PFAS Solutions, New Castle, DE*
- WP 284 **Development of a Non-target HRMS Approach for Microcystin Analysis to Bridge the Gap Between ELISA and LC-MS/MS**; Jonathan Zapata<sup>1</sup>; Matthew Prescott<sup>1</sup>; <sup>1</sup>*Metropolitan Water District, La Verne, CA*

### FUNDAMENTALS: UNCONVENTIONAL APPROACHES IN MS 285-293

- WP 285 **Fragment correlation mass spectrometry of multi-charged ions to improve molecular structural identification and resolve complex mixtures**; Yangjie Li<sup>1</sup>; Guy Cavet<sup>2</sup>; Richard N Zare<sup>1</sup>; Taran Driver<sup>1</sup>; <sup>1</sup>*Stanford University, Stanford, CA*; <sup>2</sup>*Flatiron Bio, LLC, Palo Alto, CA*
- WP 286 **Square Parametric Excitation in a Digital Linear Ion Trap**; Grace O Capek<sup>1</sup>; Etienne Garand<sup>1</sup>; <sup>1</sup>*University of Wisconsin - Madison, Madison, WI*
- WP 287 **To separate or not to separate: MS/MS fragmentation-based uncoupling of bile acid regio- and stereoisomers**; Ipsita Mohanty<sup>1</sup>; Yasin El Abiead<sup>1</sup>; Lee R. Hagey<sup>1</sup>; Pieter C. Dorrestein<sup>1</sup>; <sup>1</sup>*University of California San Diego, La Jolla, CA*
- WP 288 **Overcoming artefacts in Fourier transform-isotope ratio mass spectrometry for low abundance isotopocules**; Nils Kuhlbusch<sup>1, 2</sup>; Konstantin Aizikov<sup>3</sup>; Dmitry Grinfeld<sup>2</sup>; Dmitry Strelnikov<sup>2</sup>; Issaku E. Koh<sup>2</sup>; Dieter Juchelka<sup>2</sup>; Alexander A. Makarov<sup>2, 4</sup>; Heiko Hayen<sup>1</sup>; Andreas Hilker<sup>2</sup>; <sup>1</sup>*University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany*; <sup>2</sup>*Thermo Fisher Scientific, Bremen, Germany*; <sup>3</sup>*ThermoFisher, Bremen, Germany*; <sup>4</sup>*Utrecht University, Utrecht, Netherlands*
- WP 289 **Additively Manufactured Quadrupole Mass Filter Yields Competitive RGA Performance for a Fraction of the Production Cost**; Colin Eckhoff<sup>1</sup>; Luis F. Velasquez-Garcia<sup>1</sup>; <sup>1</sup>*MIT, Cambridge, MA*
- WP 290 **Sub-optimal conditions for enzymatic cleavage - A way to achieve maximum protein sequence coverages**; Dirk Dobritzsch<sup>1</sup>; Matthew A. Fuszard<sup>1</sup>; <sup>1</sup>*Martin-Luther-University Halle-Wittenberg, Halle, Germany*
- WP 291 **Chiral Recognition by Mass Spectrometry with the Combinations of Two Chiral Selectors**; Qi Yi; *Hong Kong Polytechnic University, Kowloon, Hong Kong*
- WP 292 **Reproducibility analysis of clinically-relevant targets identifies durable phosphopeptide ions**; Andrew Williamson<sup>1</sup>; Amy E Campbell<sup>2</sup>; Janet Kelsall<sup>3</sup>; Luis Nobre<sup>3</sup>; Pedro Moreno-Cardoso<sup>3</sup>; Weronika S Borek<sup>3</sup>; David N Perkins<sup>3</sup>; David J Britton<sup>3</sup>; Arran D Dokal<sup>3</sup>; <sup>1</sup>*Kinomica, Macclesfield, United Kingdom*; <sup>2</sup>*Kinomica Ltd, Macclesfield, United Kingdom*; <sup>3</sup>*Kinomica Ltd, Macclesfield, Cheshire, United Kingdom*
- WP 293 **Photochemical vapor generation: a tool for analyte introduction in inductively coupled plasma mass spectrometry**; Daniel LG Borges; *Federal University of Santa Catarina, Florianopolis, Brazil*

## WEDNESDAY POSTERS

### GLYCOPROTEINS I 294-324

- WP 294 **Site-Specific N-Glycosylation of Glycoproteins in Influenza Vaccines – A Study of Variability;** Zachary C Goecker<sup>1</sup>; Meghan C Burke<sup>1</sup>; Concepcion A Remoroza<sup>1</sup>; Yi Liu<sup>1</sup>; Yuri A Mirokhin<sup>1</sup>; Sergey L Sheetlin<sup>1</sup>; Dmitrii V Tchekhovskoi<sup>1</sup>; Xiaoyu Yang<sup>1</sup>; Stephen E Stein<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, Gaithersburg, MD
- WP 295 **Studying the effects of glycosylation on the entry of SARS-CoV-2 using high-mass MALDI-MS;** Yuve Zhou<sup>1,2</sup>; Congrui Tan<sup>1</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland; <sup>2</sup>KTH Royal Institute of Technology, Stockholm, Sweden
- WP 296 **A Chemoenzymatic Method for Site-Specific Profiling of Protein O-GlcNAcylation;** Longping Fu<sup>1</sup>; Ronghu Wu<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA
- WP 297 **Decipher the intricate glycoproteins from the SARS-CoV-2 family using data-independent acquisition-proton transfer charge reduction and native top-down mass spectrometry;** Weijing Liu<sup>1</sup>; Christopher Mullen<sup>1</sup>; Roberto Gamez<sup>2</sup>; Ping F. Yip<sup>2</sup>; Rosa Viner<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Lexington, MA
- WP 298 **Profiling the glycode of CD24 using a combined mass spectrometry approach;** Tim S. Veth<sup>1</sup>; Kayla A. Markuson<sup>2</sup>; Nicholas M. Riley<sup>2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA
- WP 299 **The role of N-glycans in SARS-CoV-2 Spike protein structure and cellular receptor/antibody binding;** Sarah H Osman<sup>1</sup>; John R. Barr<sup>1</sup>; Dongxia Wang<sup>1</sup>; <sup>1</sup>CDC, Chamblee, GA
- WP 300 **Characterization of offline fractionation methods for in-depth glycoproteomics;** Ruby Zhang<sup>1</sup>; Kayla A. Markuson<sup>1</sup>; Nicholas M. Riley<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- WP 301 **Enhanced surface accessibility of SARS-CoV-2 Omicron spike protein due to an altered glycosylation profile;** Dongxia Wang<sup>1</sup>; Zijian Zhang<sup>2</sup>; Jakub Baudys<sup>1</sup>; Christopher Haynes<sup>1</sup>; Sarah H. Osman<sup>1</sup>; John R Barr<sup>1</sup>; James Gumbart<sup>2</sup>; <sup>1</sup>Centers of Disease Control and Prevention (CDC), Atlanta, GA; <sup>2</sup>Georgia Tech, Atlanta, GA
- WP 302 **Tracing labeled metabolites in hypothermic CHO cells reveals a role in affecting secreted mAb quality;** Xin Bush<sup>1</sup>; Nicholas Trunfio<sup>1</sup>; Erica Berilla<sup>1</sup>; Casey Kohnhorst<sup>1</sup>; Nicole Azer<sup>1</sup>; Roberta King<sup>2</sup>; David Naoki Powers<sup>1</sup>; <sup>1</sup>FDA, Silver Spring, MD; <sup>2</sup>University of Rhode Island, Kingston, RI
- WP 303 **XIC-centric analysis recovers glycopeptide spectra missed by database searches;** Guanghui Wang<sup>1</sup>; Zheng Zhang<sup>1</sup>; Yi Liu<sup>1</sup>; Meghan C Burke<sup>1</sup>; Sergey L Sheetlin<sup>1</sup>; Stephen E Stein<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD
- WP 304 **Glycopeptide Libraries of Human Plasma Glycoproteins;** Yi Liu<sup>1</sup>; Meghan C Burke<sup>1</sup>; Sergey Sheetlin<sup>1</sup>; Goecker C Zachary<sup>1</sup>; Zheng Zhang<sup>1</sup>; Yuxue Liang<sup>1</sup>; Guanghui Wang<sup>1</sup>; Yuri A Mirokhin<sup>1</sup>; Xiaoyu Yang<sup>1</sup>; Dmitrii V Tchekhovskoi<sup>1</sup>; Stephen E Stein<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD
- WP 305 **Bottom-up glycoprotein analysis workflows including column switching, Differential Mobility Spectrometry, Electron Activation Dissociation and Ultraviolet Photodissociation;** Charlotte Jacquet<sup>1</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>University of Geneva, Geneva, Switzerland
- WP 306 **Workflow Development and Optimization for Proteomic and Glycoproteomic Analysis of Platelets;** Ying Sheng<sup>1</sup>; Yunlong Zhao<sup>1</sup>; Yuan Mao<sup>1</sup>; Ning Li<sup>1</sup>; <sup>1</sup>Regeneron Pharmaceuticals, Tarrytown, NY
- WP 307 **Utilizing novel EAD QTOF technology for bioactive protein characterization;** Greg Roman<sup>1</sup>; Dilip Reddy<sup>2</sup>; Zhengwei Chen<sup>2</sup>; Xiaoning Lu<sup>3</sup>; Lei Xiong<sup>4</sup>; <sup>1</sup>Sciex, Framingham, MA; <sup>2</sup>SCIEX, USA, Framingham, MASSACHUSETTS; <sup>3</sup>Helainia, New York, New York; <sup>4</sup>SCIEX, Redwood City, CA
- WP 308 **Characterization of the N- and O-Glycosylation of Recombinant Mpox E8 Viral Protein;** Jakub Baudys<sup>1</sup>; Theodore R. Keppel<sup>1</sup>; Yu Zhou<sup>1</sup>; John R. Barr<sup>1</sup>; Dongxia Wang<sup>1</sup>; <sup>1</sup>Centers of Disease Control and Prevention (CDC), Atlanta, GA
- WP 309 **Global O-glycoproteome enrichment and analysis enabled by a robust combinatorialenzymatic workflow;** Rohit Budhraja<sup>1</sup>; Taewook Kang<sup>1</sup>; Jinyong Kim<sup>1</sup>; Neha Joshi<sup>1</sup>; Kishore Garapati<sup>1</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Mayo clinic, Rochester, MN
- WP 310 **Cognitive Decline in Older Adults with Type 2 Diabetes: Unraveling Site-Specific N-linked Mass Spectrometry Based Glycoproteomic Alterations;** Yishai Levin<sup>1</sup>; David Morgenstern<sup>1</sup>; Hila Wolf Levy<sup>1</sup>; Barak Markus<sup>1</sup>; Itzik Cooper<sup>2</sup>; Michal Schnaider Beer<sup>3</sup>; <sup>1</sup>Weizmann Institute of Science, Rehovot, Israel; <sup>2</sup>Sheba Medical Center, Tel Hashmer, Israel; <sup>3</sup>Rutgers University, New Brunswick, NJ
- WP 311 **An Innovative Approach for Examining Disease-Related N-Glycopeptides in Small Extracellular Vesicles: A Case Study on Traumatic Brain Injury;** Ayobami O. Oluokun<sup>1</sup>; Mojibola O Fowowe<sup>1</sup>; Cristian D Gutierrez-Reyes<sup>1</sup>; Moyinoluwa Adeniyi<sup>1</sup>; Sherifdeen B Onigbinde<sup>1</sup>; Oluwatosin E Daramola<sup>1</sup>; Angel J Garcia<sup>1</sup>; Firas Kobeissy<sup>2</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA
- WP 312 **Ionization Efficiency of Homologous Saccharides in various Modes of Electrospray;** Nicholas Allen<sup>1</sup>; Ian T Ferraro<sup>1</sup>; Nancy Fernandes<sup>2</sup>; Thaddaeus Webster<sup>2</sup>; Carrie Mason<sup>2</sup>; Tolulope Ogunsanya<sup>1</sup>; Anyin Li<sup>1</sup>; <sup>1</sup>University of New Hampshire, Durham, NH; <sup>2</sup>Lonza Biologics, Portsmouth, New Hampshire
- WP 313 **Detection of Glucose-Regulated Sites of Protein O-GlcNAc Modification;** Lauren E Ball<sup>1</sup>; Mi-Hye Lee<sup>1</sup>; Jennifer R Bethard<sup>1</sup>; Rony Hull<sup>1</sup>; Susana Comte-Walters<sup>1</sup>; Mauricio J Reginato<sup>2</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC; <sup>2</sup>Drexel University, Philadelphia, PA
- WP 314 **Simultaneous Deglycosylation and Nontryptic Protease Digestion;** Jade K. Macdonald<sup>1</sup>; Richard R. Drake<sup>1</sup>; Anand S. Mehta<sup>1</sup>; Peggi Angel<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC
- WP 315 **Network method for building a sample-specific glycan database for N-linked glycosylation from MS/MS data;** Aliana Tang<sup>1</sup>; Marshall W. Bern<sup>2</sup>; <sup>1</sup>Piedmont High School, Piedmont, CA; <sup>2</sup>Protein Metrics, LLC, Cupertino, CA
- WP 316 **High-Throughput Spatial Glycoproteomics: Deciphering Age-Related Glycosylation Changes in the Mouse Brain;** Delf-Magnus Kummerfeld<sup>1, 2</sup>; Johanna Schrader<sup>3</sup>; Aleksander J. Nowak<sup>4</sup>; Joanna M. Kirkpatrick<sup>4</sup>; Peter Milland<sup>5</sup>; Eugen Damoc<sup>4</sup>; Boris V. Skryabin<sup>2</sup>; Hans H. Wandall<sup>6</sup>; Timofey S. Rozhdenskiy<sup>2</sup>; Sergey Y. Vakhrushev<sup>6</sup>; <sup>1</sup>Leibniz Institute on Aging - Fritz Lipmann Institute (FLI), Jena, Germany; <sup>2</sup>Transgenic animal and genetic engineering Models (TRAM), Core facility, Medical Faculty, Muenster University, Muenster, Germany; <sup>3</sup>L3S Research Center, Hannover, Germany; <sup>4</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; <sup>5</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>6</sup>University of Copenhagen, Department of Cellular and Molecular Medicine, Copenhagen Center for Glycomics, Copenhagen N, Denmark
- WP 317 **Differential N-Glycosylation Site Occupancy Depends on Distinct Amino Acid Sequence Features of Oligosaccharyltransferase and Acceptor Polypeptides;** Mariam Khaleque<sup>1</sup>; Amanda Nouwens<sup>2</sup>; Elisa Fadda<sup>3</sup>; Benjamin Schulz<sup>2</sup>; <sup>1</sup>Columbia University, New York, NY; <sup>2</sup>University of Queensland, Brisbane, Australia; <sup>3</sup>Maynooth University, Kildare, Ireland
- WP 318 **Large Scale Characterization of N-linked Glycopeptides from Human Serum Using HILIC Enrichment and LC-MS Analysis;** Raghavendra Rao Pasupuleti<sup>1</sup>; Jonathan C Trinidad<sup>1</sup>; <sup>1</sup>Department of Chemistry, Indiana University, Bloomington, IN, 47405
- WP 319 **Determination of Glycoform Masses of SARS-CoV-2 Spike Protein Variants by Electron Capture Charge Reduction Mass Spectrometry;** Zhixin Xu<sup>1,2</sup>; Chen Du<sup>1,2</sup>;

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- Eduardo Olmedillas<sup>3</sup>; Regina M. Edgington<sup>1</sup>; Sophie R. Harvey<sup>2</sup>; Erica Ollmann Saphire<sup>3, 4</sup>; Vicki H. Wysocki<sup>1, 2</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; <sup>2</sup>Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH; <sup>3</sup>Center for Vaccine Innovation, La Jolla Institute for immunology, La Jolla, California; <sup>4</sup>Department of Medicine, University of California, San Diego, La Jolla, California
- WP 320 **Analyzing Patterns of Sugar Fragmentation from Glycopeptide Tandem Mass Spectra;** Jonathan C. Trinidad<sup>1</sup>; Gabriel D Newton<sup>1</sup>; <sup>1</sup>Indiana University Bloomington, Bloomington, IN
- WP 321 **Method Development for Ferret IgG N-Glycosylation Profiling from serum using timsTOF Pro2;** Thao T. Nguyen<sup>1</sup>; Min Hui Guan<sup>1</sup>; Lei Li<sup>2</sup>; Brian P. Mooney<sup>1</sup>; Michael C. Greenleaf<sup>1</sup>; Xiu Feng Wan<sup>1</sup>; <sup>1</sup>University of Missouri-Columbia, Columbia, MO; <sup>2</sup>Georgia State University, Atlanta, GA
- WP 322 **Identifying Protein Carriers of  $\alpha$ 2,3 sialylated N-linked glycosylation using bioorthogonal derivatization and enrichment;** Hongxia Bai<sup>1</sup>; Peggi M Angel<sup>1</sup>; Richard R Drake<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC
- WP 323 **Intact Glycopeptide Analysis of Human Colon Cancer Tissue by High Resolution Liquid Chromatography-Tandem Mass Spectrometry;** Kathryn L. Kapp<sup>1,2</sup>; Fernando J. Garcia Marques<sup>1</sup>; Abel Bermudez<sup>1</sup>; Nikhiya Shamsher<sup>1</sup>; Scot Liu<sup>3</sup>; Jeong Kim<sup>3</sup>; Ashok Dongre<sup>4</sup>; Sharon J. Pitteri<sup>1</sup>; <sup>1</sup>Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; <sup>2</sup>Propel Postdoctoral Scholars Program, Stanford University School of Medicine, Stanford, CA; <sup>3</sup>Bristol Myers Squibb, Redwood City, CA; <sup>4</sup>Bristol Myers Squibb, Cambridge, MA
- WP 324 **Alternative glycoprotein labeling to access the intact cell surface proteome;** Emmajay Sutherland<sup>1</sup>; Nicholas M. Riley<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Washington, Seattle, WA
- HIGH THROUGHPUT MS II**  
**325-349**
- WP 325 **Improving sensitivity of acoustic-ejection mass spectrometry in biological matrices using solid-phase extraction and carrier solvent optimization;** Md Jahangir Alam<sup>1</sup>; Grace Proske<sup>1</sup>; Bernard K Choi<sup>1</sup>; Rajesh Desai<sup>1</sup>; Paul Harradine<sup>1</sup>; <sup>1</sup>Merck & Co. Inc., West Point, PA
- WP 326 **Capillary-flow sub-minute gradient LC/MS/MS for robust and ultrahigh-speed proteomics;** Ayana Tomioka<sup>1</sup>; Ryota Tomioka<sup>1</sup>; Eisuke Kanao<sup>1,2</sup>; Kosuke Ogata<sup>1</sup>; Koshi Imami<sup>3</sup>; Naoyuki Sugiyama<sup>1</sup>; Yasushi Ishihama<sup>1,2</sup>; <sup>1</sup>Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; <sup>2</sup>National Institutes of Biomedical Innovation, Health and Nutrition, Ibraki, Japan; <sup>3</sup>RIKEN Center for Integrative Medical Sciences, Yokohama, Japan
- WP 327 **High-throughput Mass Spectrometry (HTMS) Techniques for Bile Salt Export Pump (BSEP) Assay;** Jie Li<sup>1, 2</sup>; Nicolás Morato<sup>2</sup>; Lori Westover<sup>3</sup>; Pravien Abeywickrema<sup>3</sup>; Jieping Geng<sup>3</sup>; Madison Piassek<sup>3</sup>; David Harden<sup>3</sup>; Iulia Strambeanu<sup>1</sup>; Nico Vervoort<sup>4</sup>; Bo Hao<sup>1</sup>; Karel Goossens<sup>4</sup>; Zhicai Shi<sup>1</sup>; Harsha Gunawardena<sup>5</sup>; Juncai Meng<sup>3</sup>; R. Graham Cooks<sup>2</sup>; <sup>1</sup>Global Discovery Chemistry, Janssen R&D, Spring House, PA; <sup>2</sup>Department of Chemistry, Purdue University, West Lafayette, IN; <sup>3</sup>Discovery Technology and Molecular Pharmacology, Janssen R&D, Spring House, PA; <sup>4</sup>CPRD, Janssen R&D, Beerse, Belgium; <sup>5</sup>Cell Engineering & Analytical Sciences, Janssen R&D, Spring House, PA
- WP 328 **Quality control system and QC data analysis pipeline for high throughput targeted LC-MS proteomics encompassing sample quality to instrument suitability;** Jonathan T. Bui<sup>1</sup>; Chi D. L. Nguyen<sup>1</sup>; Erika Hernandez<sup>1</sup>; Dragana Noe<sup>1</sup>; Zachary Dwight<sup>1</sup>; Jennifer E. Van Eyk<sup>2</sup>; Susan Mockus<sup>1</sup>; <sup>1</sup>Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA; <sup>2</sup>Advanced Clinical BioSystems Research Institute, Cedars-Sinai Medical Center, Los Angeles, CA
- WP 329 **Comparing plate-based high-throughput proteomics approaches for plasma depletion: antibody-based resin vs perchlorate precipitation;** Nathan Hendricks<sup>1</sup>; Josselin Ortiz<sup>1</sup>; Angel Keoseyan<sup>1</sup>; Santosh D Bhosale<sup>1</sup>; Annie Moradian<sup>1</sup>; Susan Mockus<sup>1</sup>; <sup>1</sup>Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, California
- WP 330 **Characterization of Complex Cellular Signatures from Organophosphate Exposure Over Time Using Integrated Multiomic Analysis;** Tara Harvey<sup>1, 2</sup>; Emilio S. Rivera<sup>1, 2</sup>; Emilia A. Solomon<sup>2</sup>; Claire K. Sanders<sup>3</sup>; Joshua D. Breidenbach<sup>1, 2</sup>; Kes A. Luchini<sup>1, 2</sup>; Grace M. Thornhill<sup>1, 2</sup>; Brett R. Blackwell<sup>1, 2</sup>; Chi-Yen Tseng<sup>1, 2</sup>; Erick S. LeBrun<sup>1, 2</sup>; Marc Alvarez<sup>2</sup>; Abigale S Mikolitis<sup>1, 2</sup>; Bob Williams<sup>2</sup>; Zachary J. Sasiene<sup>1, 2</sup>; Ethan M. McBride<sup>1, 2</sup>; Austin R. Anderson<sup>1, 2</sup>; Lauren K. Heine<sup>1, 2</sup>; Jessica A. Salguero<sup>1, 2</sup>; Francisca E. Rodriguez<sup>1, 2</sup>; Salvador J. Palmisano<sup>1, 2</sup>; Phillip M. Mach<sup>1, 2</sup>; Trevor G. Glaros<sup>1, 2</sup>; <sup>1</sup>Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>3</sup>Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM
- WP 331 **Rapid Discovery of Medical Countermeasures against Emerging Pathogens using High-throughput DESI and 2D MS/MS;** Dalton Snyder<sup>1</sup>; Andrew Eller<sup>1</sup>; Scott Griffin<sup>1</sup>; Megan Guetzloff<sup>1</sup>; Miranda Jacobs<sup>1</sup>; Ann Donnelly<sup>1</sup>; Andrew Houvenagle<sup>1</sup>; Kevin Rosenbaum<sup>1</sup>; Austin Stieglitz<sup>1</sup>; Ilya Shinkeyev<sup>1</sup>; Kerry O'Donnell<sup>1</sup>; Brandon Reese<sup>1</sup>; Anna Leech<sup>1</sup>; Mitch Wells<sup>1</sup>; <sup>1</sup>Teledyne FLIR, West Lafayette, IN
- WP 332 **HT-Intact Covalent Binding: Analysis automation workflow for scaled multiplexed screening with stringent quality control;** Matthew Green<sup>1</sup>; Juan Florez<sup>2</sup>; Stephan Heyse<sup>2</sup>; Stephen Steigle<sup>2</sup>; <sup>1</sup>Genedata, Cambridge, United Kingdom; <sup>2</sup>Genedata, Basel, Switzerland
- WP 333 **High-throughput Acoustic Ejection Mass Spectrometry with adjustable signal durations;** Bradley Schneider<sup>1</sup>; Jing Ma<sup>2</sup>; Chiu Cheong Aw<sup>2</sup>; Heguang Ji<sup>2</sup>; Lin Shuxian<sup>2</sup>; Xuejiao Yin<sup>2</sup>; Huiyin Tey<sup>2</sup>; Chang Liu<sup>1</sup>; <sup>1</sup>SCIEX, Concord, ON; <sup>2</sup>SCIEX, Singapore, Singapore
- WP 334 **Automated online protein-ligand binding and its detection using native mass spectrometry;** Weijing Liu<sup>1</sup>; Wilson Phung<sup>2</sup>; Wendy Sandoval<sup>2</sup>; Rosa Viner<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Genentech Inc, South San Francisco, CA
- WP 335 **Life in the Fast Lane: A Rapid Screening Method for the SAMHSA Urine and Oral Fluid Drug Lists by RapidFire-MS;** Jennifer Cottine Hitchcock; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- WP 336 **Automated and High Throughput Analysis of AAV Biotherapeutics Using SampleStream and Individual Ion Mass Spectrometry;** Samuel E. Janisse<sup>1</sup>; Mike Goodwin<sup>2</sup>; Ryan T. Fellers<sup>1</sup>; Ping F. Yip<sup>2</sup>; Kristina Srzentic<sup>3</sup>; Kyle P. Bowen<sup>2</sup>; Josh Smith<sup>4</sup>; Jonathan Bones<sup>4</sup>; Michael W. Senko<sup>2</sup>; Jared O. Kafader<sup>1</sup>; Philip D. Compton<sup>5</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>Proteomics Center of Excellence, Northwestern University, Evanston, Illinois; <sup>2</sup>ThermoFisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific, Reinach, Switzerland; <sup>4</sup>National Institute for Bioprocessing Research and Training, Dublin, Ireland; <sup>5</sup>Integrated Protein Technologies, Inc, Evanston, IL
- WP 337 **Systematic Comparison of High-Throughput Activity-Based Proteomics LC-MS Methods for Quantitative Reactive Cysteine Profiling in a Cellular Context;** Violette Gautier<sup>1</sup>; Giada Marino<sup>2</sup>; Nagarjuna Nagaraj<sup>2</sup>; Pierre-Olivier Mau<sup>3</sup>; Marion Tondeur<sup>1</sup>; Guillaume Vink<sup>1</sup>; Marie Guillemot<sup>1</sup>; Navratan Bagwan<sup>1</sup>; Philipp Strohmidel<sup>4</sup>; Catherine Pech<sup>5</sup>; Francois Autelitano<sup>1</sup>; <sup>1</sup>EVOTEC, Toulouse, France; <sup>2</sup>Evotec München GmbH, Munich, Germany;

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- WP 338 <sup>3</sup>Evotec SE, Toulouse, France; <sup>4</sup>Bruker Daltonics GmbH & Co.KG, Bremen, Germany; <sup>5</sup>EVOTEC, Toulouse, France  
**Fine-tuning Mag-Net: Advancing plasma proteome profiling through parameter optimization and comparative analysis;** Adele Nel<sup>1,2</sup>; Sindisiwe Buthelezi<sup>3</sup>; Ireshyn S Govender<sup>1</sup>; Previn Naicker<sup>1,3</sup>; Andrea Ellero<sup>1,2</sup>; Stoyan Stoychev<sup>4</sup>; Justin Jordaan<sup>1</sup>; Christine Wu<sup>5</sup>; Michael J. MacCoss<sup>6</sup>; <sup>1</sup>ReSyn Biosciences, Pretoria, South Africa; <sup>2</sup>University of Pretoria, Pretoria, South Africa; <sup>3</sup>Council for Scientific and Industrial research, Pretoria, South Africa; <sup>4</sup>ReSyn BioSciences, Johannesburg, South Africa; <sup>5</sup>University of Washington, seattle, WA; <sup>6</sup>University of Washington, Seattle, WA
- WP 339 **Evaluation of Improved Methodology for Proteograph XT Nanoparticle-Enriched Plasma with ThermoFisher Orbitrap Astral Mass Spectrometer;** Lee S. Cantrell<sup>1</sup>; Eltahir Elgierari<sup>1</sup>; Jian Wang<sup>1</sup>; Gabriel Castro<sup>1</sup>; Ryan W. Benz<sup>1</sup>; Jimmy Zeng<sup>2</sup>; Bruce Wilcox<sup>2</sup>; Serafim Batzoglou<sup>1</sup>; <sup>1</sup>Seer Inc., Redwood City, CA; <sup>2</sup>Prognomiq Inc., San Mateo, California
- WP 340 **High-throughput and rapid screening of PFAS in drinking water using solid-phase microextraction with microfluidic open interface-mass spectrometry;** MALVIKA DUTT<sup>1,2</sup>; WEI ZHOU<sup>2</sup>; ACHILLE CAPPIELLO<sup>1,3</sup>; JANUSZ PAWLISZYN<sup>2</sup>; <sup>1</sup>UNIVERSITY OF URBINO CARLO BO, URBINO, Italy; <sup>2</sup>University of Waterloo, Waterloo, ON; <sup>3</sup>Vancouver Island University, Nanaimo, BC
- WP 341 **A proximity proteomics pipeline for subcellular proteome and protein interaction mapping;** Xiaofang Zhong<sup>1</sup>; Qiongyu Li<sup>1</sup>; Benjamin Polacco<sup>1</sup>; Trupti Patil<sup>1</sup>; Aaron Marley<sup>1</sup>; Helene Foussard<sup>1</sup>; Prachi Khare<sup>1</sup>; Rasika Vartak<sup>1</sup>; Jiewei Xu<sup>1</sup>; Jeffrey DiBerto<sup>2</sup>; Bryan Roth<sup>2</sup>; Manon Eckhardt<sup>1</sup>; Mark Von Zastrow<sup>1</sup>; Nevan Krogan<sup>1</sup>; Ruth Huttenhain<sup>1</sup>; <sup>1</sup>University of California-San Francisco, San Francisco, CA; <sup>2</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC
- WP 342 **Development of a High-Throughput Screening Assay to Identify Inhibitors of Plasmodium falciparum Acetyl-CoA synthetase Using RapidFire Mass Spectrometry;** De Lin<sup>1</sup>; Andrew Plater<sup>1</sup>; Joao Pisco<sup>1</sup>; Avinash Puneekar<sup>1</sup>; Andrew Shepherd<sup>1</sup>; Sharon Shepherd<sup>1</sup>; Leah Torrie<sup>1</sup>; Beatriz Baragana<sup>1</sup>; David W. Gray<sup>1</sup>; <sup>1</sup>Drug Discovery Unit, School of Life Sciences, University of Dundee, Dundee, United Kingdom
- WP 343 **Desorption Electrospray Ionization and 2D-MS/MS for High Throughput Biomolecular Analysis;** Thomas C. Sams<sup>1</sup>; Louis Edwin Gonzalez<sup>1</sup>; Sam Edward Ying<sup>1</sup>; Christina R. Ferreira<sup>1</sup>; Kai-Hung Huang<sup>1</sup>; Nicolás Morato<sup>1</sup>; Kitmin Chen<sup>1</sup>; Eric Dziekonski<sup>1</sup>; Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- WP 344 **Accelerated Late-Stage Functionalization of Opioid Drugs in Microdroplets;** Jyotirmoy Ghosh<sup>1</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN
- WP 345 **A novel tandem LC workflow for proteome analysis with near 100% MS utilization;** Runsheng Zheng<sup>1</sup>; Martin Rendl<sup>1</sup>; Tabiwang N Arrey<sup>2</sup>; Neloni Wijeratne<sup>3</sup>; Christopher Pynn<sup>1</sup>; Alec Valenta<sup>1</sup>; Ece Aydin<sup>1</sup>; Maksim Daniliuk<sup>4</sup>; Robert van Ling<sup>5</sup>; Scott M Peterman<sup>3</sup>; Eugen Damoc<sup>2</sup>; Claudia Martins<sup>3</sup>; Philip Remes<sup>3</sup>; Cristina Jacob<sup>3</sup>; Wim Decrop<sup>1</sup>; Martin Samonig<sup>1</sup>; Anne Morgenstern<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Germering, Germany; <sup>2</sup>Thermo Fisher Scientific GmbH, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA; <sup>4</sup>Thermo Fisher Scientific, Vilnius, Lithuania; <sup>5</sup>Thermo Fisher Scientific, Breda, Netherlands
- WP 346 **Accelerating Drug Discovery and Lead Optimization: Unleashing the Power of High Throughput Mass Spectrometry for Rapid Molecular Insights;** Patrick Bingham<sup>1</sup>; Karen Maegley<sup>1</sup>; Juliana Piscatelli<sup>1</sup>; John Lazzaro<sup>2</sup>; Brendon Kapinos<sup>2</sup>; Jamie Tourville<sup>2</sup>; Alandra Quinn<sup>2</sup>; Nallely Juarez-Rodriguez<sup>2</sup>; <sup>1</sup>Pfizer Inc., San Diego, CA; <sup>2</sup>Pfizer Inc., Groton, CT
- WP 347 **A Chemical Derivatization MRM Method for High-Throughput MS-Based Screening to Identify Small-Molecule Modulators of Deoxyhypusine Synthase;** Christopher A LeClair<sup>1</sup>; Dingyin Tao<sup>1</sup>; Yuhong Fang<sup>1</sup>; Ken Chih-Chien Cheng<sup>1</sup>; Wei Zhao<sup>1</sup>; Ravi Tharakan<sup>1</sup>; Shyh-Ming Yang<sup>1</sup>; Myung-Hee Park<sup>2</sup>; Matthew D Hall<sup>1</sup>; <sup>1</sup>National Center for Advancing Translational Sciences, NIH, Rockville, MD; <sup>2</sup>National Institute of Dental and Craniofacial Research, NIH, Bethesda, MD
- WP 348 **High throughput online buffer exchange native MS method for screening of protein-ligand interactions;** Mohamed Ibrahim Gadallah<sup>1</sup>; Jada N. Walker<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>University of Texas at Austin, Austin, TX
- WP 349 **High-throughput Mass Spectrometry - Based Detection of Deamination Activity of ADAR1 without Prior Separation;** Yating Wang<sup>1</sup>; Travis Pemberton<sup>1</sup>; Ping Zhang<sup>2</sup>; Iyonce Rodrigo<sup>2</sup>; Zhigang Wang<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb, Cambridge, MA; <sup>2</sup>Bristol Myers Squibb, Lawrenceville, NJ

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- WP 350 **Gel-assisted mass spectrometry imaging enables sub-micrometer spatial lipidomics;** Yat Ho Chan<sup>1</sup>; Koralege C Pathmasiri<sup>1</sup>; Dominick Pierre-Jacques<sup>1</sup>; Nannan Tao<sup>2</sup>; Joshua L. Fischer<sup>2</sup>; Ethan Yang<sup>2</sup>; Stephanie Cologna<sup>1</sup>; Ruixuan Gao<sup>1</sup>; <sup>1</sup>University of Illinois Chicago, Chicago, IL; <sup>2</sup>Bruker Daltonics, Billerica, MA
- WP 351 **Multiplexed Quantitative Imaging of Proteins Delivered by Polymeric Nanocarriers;** Teerapong Jantararat<sup>1</sup>; Dheeraj K. Agrohia<sup>1</sup>; Ritabrita Goswami<sup>1</sup>; Yağız Anıl Çiçek<sup>1</sup>; Vincent M. Rotello<sup>1</sup>; Richard W. Vachet<sup>1</sup>; <sup>1</sup>University of Massachusetts Amherst, Amherst, MA
- WP 352 **Decellularization improves MALDI-MS Imaging of Extracellular Matrix Proteins in Tissues;** Akaansha Rampal<sup>1</sup>; Ngoc Vu<sup>1</sup>; Shelly R. Peyton<sup>1</sup>; Richard W. Vachet<sup>1</sup>; <sup>1</sup>University of Massachusetts Amherst, Amherst, MA
- WP 353 **Imaging mass spectrometry of sulfatide isomers enabled by gas-phase charge inversion ion/ion reactions;** Julia R Bonney<sup>1,2</sup>; Ariana E Stratton<sup>1</sup>; Yingchan Guo<sup>1</sup>; Paul Zerebinski<sup>1</sup>; Boone M. Prentice<sup>1</sup>; <sup>1</sup>University of Florida Department of Chemistry, Gainesville, FL; <sup>2</sup>Department of Neurosurgery, Brigham and Women's Hospital, Harvard Medical School, Boston, MA
- WP 354 **3D Mass Imaging of Bacterial Biofilm Composition using Water Cluster SIMS;** Mark Duncan Mills<sup>1</sup>; Naoko Sano<sup>1</sup>; Michal Ryszkak<sup>1</sup>; Kate McHardy<sup>1</sup>; David Ward<sup>1,2</sup>; Nick A. Von Jeinsen<sup>1,2</sup>; <sup>1</sup>Ionoptika, Chandlers Ford, United Kingdom; <sup>2</sup>Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom
- WP 355 **Cryo-3D MSI for Plant cells at 90 Kelvin by Water Cluster Secondary Ion Mass Spectrometry (Cluster SIMS);** Michal Ryszkak<sup>1</sup>; Naoko Sano<sup>1</sup>; Mark Duncan Mills<sup>1</sup>; Paul Blenkinsopp<sup>1</sup>; <sup>1</sup>Ionoptika Ltd, Chandlers Ford, United Kingdom
- WP 356 **Optimizing the Detection of Neurotransmitters and Related Metabolites by IR-MALDESI-MSI Utilizing Sucrose-Embedding for the Study of Ischemic Stroke in Mouse;** Mary F Wang<sup>1</sup>; Yunxin Ouyang<sup>2</sup>; Tatiana Segura<sup>2</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>Duke University, Durham, NC
- WP 357 **Novel quantitative mass spectrometry imaging strategy using the method of standard addition;** Lucie Davidová<sup>1</sup>; Ingela Lanekoff<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden
- WP 358 **High efficiency mass spectrometry imaging using single-pixel imaging strategy;** Aojie Zhang<sup>1</sup>; Xiangyu Guo<sup>1</sup>; Wenpeng Zhang<sup>1</sup>; Zheng Ouyang<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China
- WP 359 **Enhancing Analytical Precision: Method Optimization for Robust Peptide MALDI-MSI Analysis;** Jessica K Lukowski<sup>1</sup>; Jaeyeon Kim<sup>2</sup>; Young Ah Goo<sup>2</sup>; <sup>1</sup>Washington University School of Medicine, St Louis, MO; <sup>2</sup>Washington University School of Medicine, St. Louis, MO
- WP 360 **Development of Standard Materials for MALDI MS Imaging of Tissue N-glycans and Applications to Glycosylation Dysregulation in Multiple Sclerosis;** Xuan Lan Mai<sup>1</sup>; Bozena Szulc<sup>1</sup>; William Branton<sup>1</sup>; Ling Han<sup>1</sup>; Elena N. Kitova<sup>1</sup>; Christopher Power<sup>1</sup>; Jason Plemel<sup>1</sup>; Lara K.

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- Mahal<sup>1</sup>; John S. Klassen<sup>1</sup>; <sup>1</sup>University of Alberta, Edmonton, AB
- WP 361 **MALDI Mass Spectrometry Imaging Analysis of Gene expression and Metabolomic Signatures in Alzheimer's Disease Model**; Kyle A Vanderschoot<sup>1</sup>; Jacob P. Padilla<sup>1</sup>; Kelli A. Steinneman<sup>1</sup>; Jacopo Di Lucente<sup>1</sup>; Izumi Maezawa<sup>1</sup>; Lee-way Jin<sup>1</sup>; Marie C. Heffern<sup>1</sup>; Elizabeth K Neumann<sup>1</sup>; <sup>1</sup>University of California, Davis, Davis, California
- WP 362 **On-tissue dataset-dependent MALDI-TIMS-MS2 bioimaging**; Steffen Heuckeroth<sup>1,2</sup>; Arne Behrens<sup>3</sup>; Carina Wolf<sup>2</sup>; Arne Fütterer<sup>3</sup>; Ansgar Korf<sup>1</sup>; Henning Richter<sup>4</sup>; Astrid Jeibmann<sup>5</sup>; Uwe Karst<sup>2</sup>; Robin Schmid<sup>6</sup>; <sup>1</sup>mzio GmbH, Bremen, Germany; <sup>2</sup>University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; <sup>3</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>4</sup>University of Zurich, Zürich, Switzerland; <sup>5</sup>Institute for Neuropathology, University of Muenster, Muenster, Germany; <sup>6</sup>Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic
- WP 363 **Parallel data acquisition for multiplexed mass spectrometry imaging targeting oxidized cholesterol metabolites in multiple sclerosis**; Varun Vashneel Sharma<sup>1</sup>; Gabor Toth<sup>1</sup>; Johan Lillja<sup>1</sup>; Cathrin Hansen<sup>2</sup>; Gijs Kooij<sup>2</sup>; Ingela Lanekoff<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>Amsterdam University Medical Center, Amsterdam, Netherlands
- WP 364 **A novel MALDI IMS approach for improved spatial visualization of small molecules in formalin-fixed paraffin-embedded tissue sections**; Georgia Charkoftaki<sup>1</sup>; Athina Lisgara<sup>1</sup>; Alvaro Santos-Neto<sup>1,2</sup>; Reza Aalizadeh<sup>1</sup>; Michael Becker<sup>3</sup>; Nina Gonnella<sup>4</sup>; Vladimir V Papov Jr. <sup>4</sup>; Vasilis Vasiliou<sup>1</sup>; <sup>1</sup>Yale School of Public Health, New Haven, CT; <sup>2</sup>University of São Paulo, São Carlos, Brazil; <sup>3</sup>Boehringer Ingelheim, Biberach an der Riß, Germany; <sup>4</sup>Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, Connecticut
- WP 365 **The effect of solvents on metabolomic and lipidomic recovery from formalin-fixed paraffin-embedded human brain tissue sections by DESI-MSI**; Tassia Venga Mendes<sup>1</sup>; Emily Xinlei Ma<sup>2</sup>; Patrick R. Hof<sup>3</sup>; Dan Meyer<sup>4</sup>; Samantha Abate<sup>4</sup>; Elizabeth McDonough<sup>4</sup>; Merina Varghese<sup>3</sup>; Livia S. Eberlin<sup>1</sup>; <sup>1</sup>Baylor College of Medicine, Houston, TX; <sup>2</sup>Rice University, Houston, TX; <sup>3</sup>Icahn School of Medicine at Mount Sinai, New York, NY; <sup>4</sup>GE HealthCare, Niskayuna, NY
- WP 366 **Cyclic MALDI-IHC for Successive High-plex and Multimodal Imaging of Tissues and Tissue Microarrays**; Leonardo G. Dettori<sup>1</sup>; Gargey Yagnik<sup>1</sup>; Philip Carvalho<sup>1</sup>; Mark J. Lim<sup>1</sup>; Kenneth J. Rothschild<sup>1,2</sup>; <sup>1</sup>AmberGen Inc., Billerica, MA; <sup>2</sup>Boston University, Department of Physics and Photonics Center, Boston, MA
- WP 367 **Tuning MSI for Deeper Spatial Proteomics in Drug Discovery: Matrix Enhancing Charge State and Search Algorithm Design for IM-MS Bias**; Emily R. Sekera<sup>1</sup>; Xusheng Wang<sup>1</sup>; Yingxue Fu<sup>1</sup>; Anthony High<sup>1</sup>; Zoran Rankovic<sup>1</sup>; John J. Bowling<sup>1</sup>; <sup>1</sup>St. Jude Children's Research Hospital, Memphis, TN
- WP 368 **Optimization of liquid extraction surface analysis (LESA) for microenvironments within Pseudomonas aeruginosa biofilms**; Dharmeshkumar Parmar<sup>1,2</sup>; Abigail Weaver<sup>3</sup>; Joshua D Shrout<sup>3,4</sup>; Jonathan V Sweedler<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, University of Illinois Urbana-Champaign, Champaign, IL; <sup>2</sup>Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Champaign, IL; <sup>3</sup>Department of Biological Sciences, University of Notre Dame, Notre Dame, Indiana; <sup>4</sup>Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, Notre Dame, Indiana
- WP 369 **Mass spectrometry imaging detection of counterfeits and forgery**; Veronika Tibljas<sup>1</sup>; Robert Bradshaw<sup>1</sup>; Simona Francese<sup>1</sup>; Marjory Da Costa Abreu<sup>1</sup>; <sup>1</sup>Sheffield Hallam University, Sheffield, United Kingdom
- WP 370 **Combination of fluorescence and IR images with protein and lipid MALDI Imaging allows more insights into disease phenotypes**; Corinna Henkel<sup>1</sup>; Bjoern Wendik<sup>1</sup>; Tanja Bien<sup>1</sup>; Bram Heijs<sup>1</sup>; Arne Behrens<sup>1</sup>; David Ahlers<sup>2</sup>; Jan Schwenzfeier<sup>3</sup>; Tobias Boskamp<sup>1</sup>; Soeren-Oliver Deininger<sup>1</sup>; Jens Christmann<sup>4</sup>; Uwe Karst<sup>2</sup>; Jens Soltwisch<sup>3</sup>; Andrea Tannapfel<sup>4</sup>; Savannah Snyder<sup>5</sup>; Katherine A. Stumpo<sup>5</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; <sup>2</sup>Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany; <sup>3</sup>Institute of Hygiene, University of Münster, Münster, Germany; <sup>4</sup>Institute for Pathology, Ruhr-University Bochum, Bürkle-de-la-Camp-Platz 1, 44789 Bochum, Germany; <sup>5</sup>Bruker Scientific, LLC, Billerica, MA
- WP 371 **MALDI-imaging of tryptic peptides: Improvements in spatial resolution in mammalian tissue and first applications in plants and ecotoxicological model organisms**; Bastian Jahreis<sup>1</sup>; Julia Kokesch-Himmelreich<sup>1</sup>; Oliver Wittek<sup>1</sup>; Andreas Römpf<sup>1</sup>; <sup>1</sup>Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany
- WP 372 **Enhancing a Statistics-Based System Suitability Testing Approach for Mass Spectrometry Imaging with Improved Sampling Methods and a Diverse Analyte Panel**; Quinn Mills<sup>1</sup>; Russell R Kibbe<sup>1</sup>; Alexandria L. Sohn<sup>1</sup>; Emily C Hector<sup>2</sup>; Andrew J Percy<sup>3</sup>; Krista Backiel<sup>3</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>Department of Statistics, North Carolina State University, Raleigh, NC; <sup>3</sup>Cambridge Isotope Laboratories, Tewksbury, Massachusetts
- WP 373 **Combining metabolite imaging mass spectrometry with multiplex confocal immunofluorescence microscopy for a multi-modal lymphoid tissue analysis pipeline**; Benjamin L. Oyler<sup>1</sup>; Adam Molyvdas<sup>1</sup>; Jeferson A. Valencia-Dávila<sup>1</sup>; Bindesh Shrestha<sup>2</sup>; Constantinos Petrovas<sup>3</sup>; Amina Woods<sup>1</sup>; Richard Koupi<sup>1</sup>; <sup>1</sup>NIH, Gaithersburg, MD; <sup>2</sup>Waters Corporation, Milford, Massachusetts; <sup>3</sup>University of Lausanne, Lausanne, Switzerland
- WP 374 **Sublimated/annealed aminated cinnamic acid analogues for high sensitivity 3 µm spatial resolution MALDI IMS of lipids in human tissues**; Martin Dufresne<sup>1</sup>; David M. G. Anderson<sup>1</sup>; Lukasz Migas<sup>2</sup>; Cody R Marshall<sup>1</sup>; Katerina V Djambazova<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; Raf Van De Plas<sup>2</sup>; Jeffrey M Spraggins<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands
- WP 375 **Metabolome profiling of mammalian tissue using varied mass spectrometry techniques for confident spatial identification**; Rosalie Chu<sup>1</sup>; Marija Velickovic<sup>1</sup>; Dusan Velickovic<sup>1</sup>; William Kew<sup>1</sup>; Karl K. Weitz<sup>1</sup>; Tujin Shi<sup>1</sup>; Tao Liu<sup>1</sup>; <sup>1</sup>PNNL, Richland, WA
- WP 376 **Multimodal Omics Imaging of Human Brain Using MALDI HiPLEX-IHC**; Yumiko Toyama<sup>1</sup>; Takashi Nirasawa<sup>2</sup>; Shigeo Murayama<sup>3</sup>; Yuko Saito<sup>3</sup>; Maho Morishima<sup>3</sup>; Masaya Ikegawa<sup>4</sup>; <sup>1</sup>Doshisha University, Kyotanabe Kyoto, Japan; <sup>2</sup>Bruker Japan K.K., Yokohama, Japan; <sup>3</sup>The Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Tokyo, Japan; <sup>4</sup>Doshisha University, Kyoto, Japan
- WP 377 **MnM: Co-spatial tissue imaging using MALDI and MIBI**;  Davide G. Franchina<sup>1</sup>; Marc Bosse<sup>1</sup>; Sam Kimmey<sup>2</sup>; Michael Angelo<sup>1</sup>; Sean Bendall<sup>1</sup>; <sup>1</sup>Stanford School of Medicine, Palo Alto, CA; <sup>2</sup>Ionpath, Menlo Park, CA
- WP 378 **Hybrid Imaging Analyses of Brain Tissue: Toward the Brain Atlas of Molecules, Elements and Metals**; Tadayuki Ogawa<sup>1</sup>; Eisei Tanaka<sup>2</sup>; Shino Takeda-Homma<sup>3</sup>; Takafumi Hirata<sup>2</sup>; Tomonari Umemura<sup>4</sup>; <sup>1</sup>Dokkyo Medical University, Mibu-machi, Japan; <sup>2</sup>The University of Tokyo, Bunkyo-ku, Japan; <sup>3</sup>National Institute of Quantum Science and Technology, Inage, Japan; <sup>4</sup>Tokyo University of Pharmacy and Life Science, Hachioji, Japan
- WP 379 **MALDI Imaging of Lipids using Long-chain n-Alkyl Primary Ammonium and Conventional Matrix Conjugate Base Organic Salt Matrices**; Brandy Perkins<sup>1</sup>; Taylor Bell<sup>1</sup>;

## WEDNESDAY POSTERS

- Kermit K. Murray<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA
- WP 380 **Protocol for quantitative mass spectrometry imaging applied to samples with spatial heterogeneity**; Reza Shariatgorji<sup>1</sup>; Anna Nilsson<sup>1</sup>; Michael Niehues<sup>1</sup>; Tina Angerer<sup>1</sup>; Per Svenningsson<sup>2</sup>; Per E. Andren<sup>3</sup>; <sup>1</sup>Uppsala university, Uppsala, Sweden; <sup>2</sup>Karolinska Institutet, Stockholm, Sweden; <sup>3</sup>Uppsala University, Uppsala, Sweden
- WP 381 **Dissecting Cerebral Amyloid Angiopathy (CAA) and Alzheimer's Disease (AD) brains with X-ray Phase-contrast microtomography combined with MALDI-Mass Spectrometry Imaging**; Rikuya Yoshimura<sup>1</sup>; Masato Hoshino<sup>2</sup>; Yumiko Toyama<sup>3</sup>; Takashi Nirasawa<sup>3</sup>; Yuko Saito<sup>4</sup>; Shigeo Murayama<sup>4</sup>; Masaya Ikegawa<sup>1</sup>; <sup>1</sup>Doshisha University, Kyoto, Japan; <sup>2</sup>Japan Synchrotron Radiation Research Institute (JASRI/SPring-8), Hyogo, Japan; <sup>3</sup>Bruker Japan K.K., Yokohama, Japan; <sup>4</sup>The Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Tokyo, Japan
- WP 382 **Design of a Novel Velocity-selected Spatial Map Ion Imaging Mass Spectrometer using SIMION**; Eric J. Smoll Jr.<sup>1</sup>; David W. Chandler<sup>1</sup>; Brian D. Patterson<sup>1</sup>; Christopher J. Kliewer<sup>1</sup>; <sup>1</sup>Sandia National Labs, Livermore, CA
- WP 383 **Evaluation of ocular distribution of low molecular drug in mouse by MALDI mass spectrometry imaging**; Hiroyuki Yokoi<sup>1</sup>; Yasuhiro Takeji<sup>2</sup>; Takeshi Fukuhara<sup>2</sup>; Ryo Doyama<sup>2</sup>; Takumi Yasuno<sup>1</sup>; Masakazu Shibata<sup>1</sup>; Yosuke Kaneko<sup>1</sup>; <sup>1</sup>Otsuka Pharmaceutical Co., Ltd, Tokushima City, Japan; <sup>2</sup>Otsuka Pharmaceutical Co., Ltd, Minoh City, Japan
- INFORMATICS: PROTEIN ID AND QUANTIFICATION**  
 384-396
- WP 384 **Enhancing Proteoform Characterization in Top-Down Mass Spectrometry Using Internal Fragment Ions**; Arthur Grimaud<sup>1</sup>; Masa Babovic<sup>1</sup>; Frederik Haugaard Vrdlovec Holck<sup>1</sup>; Ole Nørregaard Jensen<sup>1</sup>; Veit Schwämmle<sup>1</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark
- WP 385 **Quantifying proteoforms in bottom-up proteomics data using tree-based quantification**; Constantin Ammar<sup>1</sup>; Marvin Thielert<sup>1</sup>; Eugenia Voytik<sup>1</sup>; Caroline Weiss<sup>1</sup>; Edwin Rodriguez<sup>1</sup>; Maximilian T. Strauss<sup>2</sup>; Florian Rosenberger<sup>1</sup>; Wen-Feng Zeng<sup>1</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>Max Planck Institute of Biochemistry, Planegg, Germany; <sup>2</sup>Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark
- WP 386 **QuavaProt: Prediction of Variant Peptide for Screening and Quantitation via Mass Spectrometry**; Constantinos Blidijos<sup>1</sup>; Yassene Mohammed<sup>2, 3, 4</sup>; Pallab Bhowmick<sup>2</sup>; Vincent R. Richard<sup>2</sup>; Christoph H. Borchers<sup>2, 4, 5, 6</sup>; <sup>1</sup>Department of Oncology, McGill University, Montreal, QC; <sup>2</sup>Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; <sup>3</sup>Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; <sup>4</sup>Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; <sup>5</sup>Division of Experimental Medicine, McGill University, Montreal, QC; <sup>6</sup>Department of Pathology, McGill University, Montreal, QC
- WP 387 **Development of a novel Sf9 database for monitoring host cell proteins (HCPs) on Sf9-derived adeno-associated viruses (AAVs)**; Josh Smith<sup>1</sup>; Marina Ainciburu<sup>1</sup>; Ioanna Tzani<sup>1</sup>; Aaron Richardson<sup>1</sup>; Michelle Chain<sup>1</sup>; Sara Carillo<sup>1</sup>; Eugen Damoc<sup>2</sup>; Colin Clarke<sup>1, 3</sup>; Jonathan Bones<sup>1, 3</sup>; <sup>1</sup>The National Institute for Bioprocessing Research & Training, Dublin, Ireland; <sup>2</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; <sup>3</sup>School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland
- WP 388 **proteoDA: an R package for quantitative proteomics**; Charity Washam<sup>1</sup>; Duah Alkam<sup>1</sup>; Allen Gies<sup>1</sup>; Kalyani Dhusia<sup>1</sup>; Michael Robeson, II<sup>1</sup>; Stephanie Byrum<sup>1</sup>; <sup>1</sup>University of Arkansas for Medical Sciences, Little Rock, AR
- WP 389 **From CsoDIAq to zoDIAq: Applying computer science coding standards to a complete python DIA-MS proteomic data analysis software**; Caleb Cranney<sup>1</sup>; Alexandre Hutton<sup>1</sup>; Jesse Meyer<sup>1</sup>; <sup>1</sup>Cedars-Sinai Medical Center, Los Angeles
- WP 390 **Performance of LPGF Protein Validation in diverse sample types and mass spectrometry workflows**; Pedro Navarro<sup>1</sup>; Waqas Nasir<sup>1</sup>; Kai Fritzeimer<sup>1</sup>; Gorka Prieto<sup>2</sup>; Víctor M Guerrero-Sánchez<sup>3</sup>; Jesús Vázquez<sup>3</sup>; Christoph Henrich<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; <sup>2</sup>Department of Communications Engineering, University of the Basque Country (UPV/EHU), Bilbao, Spain; <sup>3</sup>Centro Nacional de Investigaciones Cardiovasculares Carlos III (CNIC), Madrid, Spain
- WP 391 **Improving Protein Identification Utilizing Various Chromatographic Methods and Multiple Search Engines**; Jesus D Castano<sup>1, 2</sup>; Francis Beaudry<sup>1, 2</sup>; <sup>1</sup>Département de Biomédecine Vétérinaire, Faculté de Médecine Vétérinaire, Université de Montréal, Montréal, Quebec; <sup>2</sup>Centre de recherche sur le cerveau et l'apprentissage (CIRCA), Université de Montréal, Montréal, Quebec
- WP 392 **TopDIA: Proteoform Identification by Top-Down Data-Independent Acquisition Proteomics**; Abdul Rehman Basharat<sup>1</sup>; Xingzhao Xiong<sup>2</sup>; Tian Xu<sup>3</sup>; Yong Zang<sup>4</sup>; Liangliang Sun<sup>3</sup>; Xiaowen Liu<sup>2</sup>; <sup>1</sup>Indiana University Purdue University Indianapolis, Indianapolis, IN; <sup>2</sup>Tulane University, New Orleans, LA; <sup>3</sup>Michigan State University, Department of Chemistry, East Lansing, MI; <sup>4</sup>Indiana University School of Medicine, Indianapolis, IN
- WP 393 **Protein identification based on Embedding Vectors Searching**; Leiver Campeon<sup>1</sup>; Sebastián Franco Gómez<sup>1</sup>; Mihira Kasun<sup>1</sup>; Lalin Theverapperuma<sup>1</sup>; Andi Krupke<sup>1</sup>; <sup>1</sup>Expert Intelligence, Santa Clara, CA
- WP 394 **A Novel Real-Time Computational Assessment of Protein Differential Expression During Mass Spectrometry Experiments for Optimization of Data Acquisition**; Aarthie Senathirajah<sup>1</sup>; Yun-En Chung<sup>1</sup>; Amit Scheer<sup>1, 2</sup>; Jonathan R. Krieger<sup>3</sup>; Tharan Srikumar<sup>3</sup>; Daniel Figeys<sup>1</sup>; Theodore J. Perkins<sup>1, 4</sup>; Mathieu Lavallée-Adam<sup>1</sup>; <sup>1</sup>University of Ottawa, Ottawa, ON; <sup>2</sup>Harvard University, Cambridge, MA; <sup>3</sup>Bruker Ltd., Milton, ON; <sup>4</sup>Ottawa Hospital Research Institute, Ottawa, ON
- WP 395 **ProteoSynth: A Tool for Ground Truth Benchmarking of Proteomics Data Processing Pipelines**; Matthew N. Dailey<sup>1</sup>; Dmitry Avtonomov<sup>1</sup>; Eric Kim<sup>1</sup>; Chris Wilkins<sup>1</sup>; Stefanie Kairs<sup>1</sup>; Sangtae Kim<sup>1</sup>; <sup>1</sup>Bertis Bioscience, SAN DIEGO, CA
- WP 396 **Ab-Twister: Fast and accurate de novo sequencing of monoclonal antibodies**; Kira Vyatkin<sup>1</sup>; Sechenov<sup>1</sup>; <sup>1</sup>University, Moscow, Russian Federation
- INFORMATICS: WORKFLOW AND DATA MANAGEMENT**  
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- WP 397 **The PRIDE Crosslinking resource: Improving FAIR data practices for crosslinking datasets**; Suresh Chanaka Hewapathirana<sup>1</sup>; Colin Combe<sup>2</sup>; Lutz Fischer<sup>3</sup>; Marcus Bage<sup>4</sup>; Sameer Velankar<sup>1</sup>; Juri Rappsilber<sup>2, 3</sup>; Yasset Perez-Riverol<sup>1</sup>; Juan Antonio Vizcaíno<sup>1</sup>; <sup>1</sup>EMBL-EBI, Hinxton, United Kingdom; <sup>2</sup>University of Edinburgh, School of Biological Sciences, Edinburgh, United Kingdom; <sup>3</sup>Technische Universität Berlin, Berlin, Germany; <sup>4</sup>EMBL-EBI, Hinxton, United Kingdom
- WP 398 **QCactus: interactive quality control software for statistical analysis and reporting metrics of raw proteomics data**; Zachary L. Dwight<sup>1</sup>; Nathan Hendricks<sup>1</sup>; Santosh D Bhosale<sup>1</sup>; Jonathan T Bui<sup>1</sup>; Monica Ghaly<sup>1</sup>; Susan M Mockus<sup>1</sup>; <sup>1</sup>Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA
- WP 399 **KPOP: a standardized data repository for open access proteomics data**; Seungjin Na<sup>1</sup>; Hokeun Kim<sup>2</sup>; Jingsi Bae<sup>2</sup>; Heeyoun Hwang<sup>1</sup>; Shinyeong Ju<sup>3</sup>; Cheolju Lee<sup>3</sup>; Jin Young Kim<sup>1</sup>; Sang-Won Lee<sup>2</sup>; Eunok Paek<sup>4</sup>; <sup>1</sup>Korea Basic Science Institute, Cheongju, South Korea; <sup>2</sup>Korea University, Seoul, South Korea; <sup>3</sup>Korea Institute of Science and Technology, Seoul, South Korea; <sup>4</sup>Hanyang University, Seoul, South Korea



## WEDNESDAY POSTERS

- WP 400 **Efficient Web Processing of Complex, Highly Dense LC/UV/MS Data Using High-Performance Computing Technologies;** Richard Lee<sup>1</sup>; Rostislav Pol<sup>1</sup>; Sofya Chudova<sup>1</sup>; <sup>1</sup>ACD/Labs, Toronto, ON
- WP 401 **A downstream proteomics analysis and visualization platform with modular design, web-interface, and persistent storage;** Pierre Jean Beltran<sup>1</sup>; Liang Xue<sup>1</sup>; Robert V Stanton<sup>1</sup>; <sup>1</sup>Pfizer, Inc, Cambridge, MA
- WP 402 **Hive: New File Format for Mass Spectrometry Measurement Data and Reader API;** Ipputa Tada<sup>1</sup>; Kazuto Mannen<sup>1</sup>; Mitsuhiro Kanazawa<sup>1</sup>; Atsushi Ogiwara<sup>1</sup>; <sup>1</sup>Reifycs Inc., Tokyo, Japan
- WP 403 **A standardized workflow for extracting and storing MS1 isotope distribution information from LC-MS proteomics experiments;** Frédérique Vilenne<sup>1</sup>; Annelies Agten<sup>1</sup>; Dirk Valkenborg<sup>1</sup>; <sup>1</sup>Hasselt University, Hasselt, Belgium
- WP 404 **QuaProt LIMS: a laboratory information management system for targeted proteomics assay development process;** Pallab Bhowmick<sup>1</sup>; Yassene Mohammed<sup>1, 2, 3</sup>; Christoph H. Borchers<sup>1, 3, 4, 5</sup>; <sup>1</sup>Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; <sup>2</sup>Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; <sup>3</sup>Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; <sup>4</sup>Division of Experimental Medicine, McGill University, Montreal, QC; <sup>5</sup>Department of Pathology, McGill University, Montreal, QC
- WP 405 **New automation tool to remotely submit LC-MS data acquisition and processing for biopharmaceutical applications;** Stephane Houel<sup>1</sup>; Kevin Schauer<sup>2</sup>; Sega Ndiaye<sup>3</sup>; Jennifer Sutton<sup>4</sup>; Tara Schroeder<sup>5</sup>; Shannon Eliuk<sup>6</sup>; <sup>1</sup>Thermo Fisher Scientific, Lexington, MA; <sup>2</sup>Thermo Fisher Scientific, Bannockburn, IL; <sup>3</sup>Thermo Fisher Scientific, Courtaboeuf, France; <sup>4</sup>ThermoFisher Scientific, San Jose, CA; <sup>5</sup>Thermo Fisher Scientific Inc, Somerset, New Jersey; <sup>6</sup>Thermo Fisher Scientific, San Jose, CA
- WP 406 **MSDMS: An Open Source Web Application to Design and Manage Custom Tandem Mass Spectrometry Libraries;** Quentin Rouchon<sup>1, 2</sup>; Gérard Hopfgartner<sup>1</sup>; <sup>1</sup>LSMS, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; <sup>2</sup>Swiss Institute of Bioinformatics (SIB), Lausanne, Switzerland
- WP 407 **Cloud-based parallelization leads to a drastically faster library-free analysis in Spectronaut;** Grzegorz Skoraczynski<sup>1</sup>; Soham Garg<sup>2</sup>; Oliver M. Bernhardt<sup>1</sup>; Damiano Robbiani<sup>1</sup>; Amy Mann<sup>2</sup>; Tejas Gandhi<sup>1</sup>; Lukas Reiter<sup>1</sup>; <sup>1</sup>Biognosys AG, Schlieren, Switzerland; <sup>2</sup>Amazon Web Services, Seattle, WA
- WP 408 **An infinite well: harmonizing all public proteomics data for machine learning;** Siegfried Gessulat<sup>1</sup>; Vishal Sukumar<sup>2</sup>; Michael Graber<sup>2</sup>; Markus Schneider<sup>2</sup>; Alexander Hogrebe<sup>1</sup>; Samia Ben Fredj<sup>2</sup>; Lizi Mamisashvili<sup>2</sup>; Tobias Schmidt<sup>2</sup>; Daniel P Zolg<sup>2</sup>; Martin Frejno<sup>2</sup>; <sup>1</sup>MSAID, Berlin, Germany; <sup>2</sup>MSAID, Garching, Germany
- WP 409 **MetaboLights - Open Access Metabolomics Resource;** Noemi Tejera<sup>1</sup>; Felix Xavier Amaladoss<sup>1</sup>; Callum Martin<sup>1</sup>; Thomas Payne<sup>1</sup>; Mark Williams<sup>1</sup>; Ozgur Yurekten<sup>1</sup>; Claire O'Donovan<sup>1</sup>; <sup>1</sup>EMBL-EBI, Hinxton, United Kingdom
- WP 410 **MassIVE: enhancing public data accessibility through extensions to the Universal Spectrum Identifier standard;** Jeremy Carver<sup>1, 2</sup>; Nuno Bandeira<sup>1, 2, 3, 4</sup>; <sup>1</sup>University of California San Diego, La Jolla, CA; <sup>2</sup>Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; <sup>3</sup>Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; <sup>4</sup>Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA
- WP 411 **Enhanced usability in the MSstats family of statistical analysis software for quantitative mass spectrometry-based proteomics;** Devon Kohler<sup>1</sup>; Mateusz Staniak<sup>2</sup>; Deril Raju<sup>1</sup>; Sarah Szvetecz<sup>1</sup>; Anthony Wu<sup>1</sup>; Olga Vitek<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>University of Wroclaw, Wroclaw, Poland
- WP 412 **Efficient Processing of Large-Scale Data-Independent Acquisition Mass Spectrometry Proteomics Experiments Using Parallelized Cloud-Native Pipelines;** Andrew Nichols<sup>1</sup>; Seth Just<sup>2</sup>; Iman Mohtashemi<sup>1</sup>; Lee Cantrell<sup>3</sup>; Jian Wang<sup>1</sup>; Harendra Guturu<sup>1</sup>; János Kis<sup>1</sup>; Yuandan Lou<sup>1</sup>; Theodore Platt<sup>1</sup>; Serafim Batzoglou<sup>1</sup>; <sup>1</sup>Seer, Inc., Redwood City, CA; <sup>2</sup>Seer, Inc, Redwood City, CA; <sup>3</sup>Seer Inc., Redwood City, CA
- WP 413 **PyC2MC: A novel software platform for the automated analysis of LC-HRMS data of complex mixtures;** Germain Salvato Vallverdu<sup>1, 2</sup>; Carlos Celis Cornejo<sup>2, 3</sup>; Martha L Chacon-Patino<sup>2, 4</sup>; Christopher Rüger<sup>5</sup>; Julien Maillard<sup>2, 6</sup>; Carlos Afonso<sup>2, 7</sup>; Christopher L Hendrichson<sup>4</sup>; Brice Bouyssiere<sup>2, 3</sup>; Pierre Giusti<sup>2, 6</sup>; Ryan P Rodgers<sup>4, 8</sup>; <sup>1</sup>Université de Pau et des Pays de l'Adour, Pau Cedex 9, France; <sup>2</sup>International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France; <sup>3</sup>Université de Pau et des Pays de l'Adour, Pau, France; <sup>4</sup>National High Magnetic Field Laboratory, Tallahassee, Florida; <sup>5</sup>University of Rostock, Rostock, Germany; <sup>6</sup>TotalEnergies, Harfleur, France; <sup>7</sup>COBRA UMR 6014, Rouen, France; <sup>8</sup>International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Tallahassee, Florida
- WP 414 **Empower your proteomics research: streamline integration, automation, and analysis with MD 2.0 Dataset Service;** Anna Quagliari<sup>1</sup>; Aaron Triantafyllidis<sup>1</sup>; Bradley Green<sup>1</sup>; Mark Condina<sup>1, 2</sup>; Paula Burton Ngov<sup>1</sup>; Giuseppe Infusini<sup>1</sup>; Andrew Webb<sup>1, 3, 4</sup>; <sup>1</sup>Mass Dynamics, Melbourne, Australia; <sup>2</sup>University of South Australia, Adelaide, Australia; <sup>3</sup>WEHI, Parkville, Australia; <sup>4</sup>University of Melbourne, Parkville, Australia
- WP 415 **Significantly faster library-free dia-PASEF analysis with a Spectronaut integrated workflow in ProteoScape;** Grzegorz Skoraczynski<sup>1</sup>; Tejas Gandhi<sup>1</sup>; Oliver M Bernhardt<sup>1</sup>; Lukas Reiter<sup>1</sup>; Sven Brehmer<sup>2</sup>; Javier Lopez<sup>2</sup>; Heidi Vitrac<sup>2</sup>; Jose Abuin<sup>2</sup>; Tharan Sri Kumar<sup>2</sup>; Dennis Trede<sup>3</sup>; <sup>1</sup>Biognosys, Zurich, Switzerland; <sup>2</sup>Bruker Daltonics Inc., Billerica, MA; <sup>3</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- WP 416 **A Comprehensive Analysis Pipeline for Phosphoproteomic Biomarker Discovery;** David N. Perkins<sup>1</sup>; Pedro Moreno-Cardoso<sup>1</sup>; Nazrath Nawaz<sup>1</sup>; Weronika E. Borek<sup>1</sup>; Josie A. Christopher<sup>1</sup>; Amy E. Campbell<sup>1</sup>; Andrew Williamson<sup>1</sup>; Arran D. Dokal<sup>1</sup>; <sup>1</sup>Kinomica Ltd, Macclesfield, Cheshire, United Kingdom
- WP 417 **BioLadder: a bioinformatic platform primarily focused on proteomic data analysis;** Yupeng Zhang<sup>1</sup>; Lixin Wang<sup>1</sup>; Jinhao Wang<sup>1</sup>; Yunping Zhu<sup>2</sup>; Songfeng Wu<sup>1</sup>; Jingli Li<sup>1</sup>; <sup>1</sup>Beijing Qinglian Biotech Co., Ltd., Beijing, China; <sup>2</sup>State Key Laboratory of Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences (Beijing), Beijing Institute of Lifeomics, Beijing, China
- WP 418 **Streamlining PRM Method Development: A Novel Computational Interface;** Jaebyeon Kim<sup>1</sup>; Minsoo Son<sup>1</sup>; Young Ah Goo<sup>1</sup>; <sup>1</sup>Mass Spectrometry Technology Access Center at McDonnell Genome Institute (MTAC@MGI) at Washington University School of Medicine, St. Louis, Missouri 64110
- WP 419 **Developing a regulatory compliant solution for nominal and accurate mass LC-MS spectrometry analysis in oligonucleotide therapeutics;** Kosuke Uchiyama<sup>1</sup>; Risa Suzuki<sup>1</sup>; Noriko Kato<sup>1</sup>; Yuka Fujito<sup>1</sup>; Neil J Loftus<sup>2</sup>; Simon Ashton<sup>2</sup>; Stephane Moreau<sup>3</sup>; <sup>1</sup>Shimadzu Corporation, Nakagyo-ku, Japan; <sup>2</sup>Shimadzu MS/BU, Manchester, United Kingdom; <sup>3</sup>Shimadzu Europa GmbH, Duisburg, Germany
- WP 420 **Thermal Proteome Profiling Analysis using FragPipe Platform;** Carolina Rojas Ramirez<sup>1</sup>; Alexey I. Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, Michigan
- WP 421 **The sky is the limit: a cloud-based proteomics platform for the masses;** Daniel P Zolg<sup>1</sup>; Markus Schneider<sup>1</sup>; Patroklos Samaras<sup>1</sup>; Samia Ben Fredj<sup>1</sup>; Florian Seefried<sup>1</sup>; Dulguun Bold<sup>1</sup>; Layla Eljagh<sup>1</sup>; Michelle Tamara Berger<sup>1</sup>;

## WEDNESDAY POSTERS

- Alexander Högrebé<sup>1</sup>; Siegfried Gessulat<sup>1</sup>; Tobias Schmidt<sup>1</sup>; Martin Frejno<sup>1</sup>; <sup>1</sup>MSAID, Garching, Germany
- WP 422 **Longitudinal data quality monitoring enables improvement of quality management practices: a case study in proteomic research utilizing a digital-twin approach**; Tharan Sri Kumar<sup>1</sup>; Cassandra Wong<sup>2</sup>; Brendon Seale<sup>2</sup>; Torsten Michael Mueller<sup>3</sup>; Stefan Harsdorf<sup>4</sup>; Sergio Legaz<sup>5</sup>; Jonathan Krieger<sup>1</sup>; Dennis Trede<sup>4</sup>; Anne-Claude Gingras<sup>2</sup>; Matthew R Lewis<sup>6</sup>; <sup>1</sup>Bruker Ltd., Milton, ON; <sup>2</sup>Lunenfeld-Tanenbaum Research Institute Mount Sinai Hospital, Toronto, Ontario; <sup>3</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>4</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>5</sup>Bruker Daltonics GmbH & Co. KG, Billerica, MA; <sup>6</sup>Bruker UK Limited, Life Sciences Mass Spectrometry Division, Coventry, United Kingdom
- WP 423 **Streamlining Protein Complex Composition Analysis with an Integrated Informatics Workflow**; Daisha Utley<sup>1</sup>; Joseph B. Greer<sup>1,2</sup>; Kenneth R. Durbin<sup>1</sup>; Ryan T. Fellers<sup>1,2</sup>; Matthew T. Robey<sup>1</sup>; Neil L. Kelleher<sup>1,2</sup>; <sup>1</sup>Proteinaceous, Inc., Evanston, IL; <sup>2</sup>Northwestern University, Evanston, IL
- WP 424 **ProteomicsDB: Connecting proteomes across species**; Armin Soleymaniya<sup>1,2</sup>; Miriam Abele<sup>3,4</sup>; Sarah Brajkovic<sup>2,4</sup>; Christina Ludwig<sup>2,3</sup>; Bernhard Kuster<sup>2,3,4</sup>; Mathias Wilhelm<sup>1,2</sup>; <sup>1</sup>Computational Mass Spectrometry, TUM, Freising, Germany; <sup>2</sup>Elite Network Bavaria, TUM, Freising, Germany; <sup>3</sup>Bavarian Center for Biomolecular Mass Spectrometry, TU Munich, TUM School of Life Sciences, Freising, Germany; <sup>4</sup>Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany
- WP 425 **Integrated Data Analysis of Oligonucleotide Therapeutics Using LC-MS, LC-MS/MS and MALDI techniques**; Nishi Rochelle<sup>1</sup>; Neil J Loftus<sup>2</sup>; Simon Ashton<sup>2</sup>; Kosuke Uchiyama<sup>3</sup>; Risa Suzuki<sup>3</sup>; Takashi Nishikaze<sup>3</sup>; Yuka Fujito<sup>3</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>2</sup>Shimadzu MS/BU, Manchester, United Kingdom; <sup>3</sup>Shimadzu Corporation, Nakagyo-ku, Japan
- WP 426 **MiCId GUI: The Graphical User Interface for MiCId, a Fast Microorganism Classification and Identification Workflow with Accurate Statistics and High Recall**; Aleksey Y Ogurtsov<sup>1</sup>; Gelio Alves<sup>2</sup>; Yi-Kuo Yu<sup>2</sup>; <sup>1</sup>CBB NCBI NLM NIH, Bethesda, MD; <sup>2</sup>NIH, Bethesda, MD
- WP 427 **ASMS 2024 Abstract: Automated Analysis of Large-Scale Proteomics Datasets Using a Data-Analysis Platform, ProEPIC**; Ajay Bharadwaj<sup>1</sup>; Niveda Sundararaman<sup>2,3</sup>; Zachary Dwight<sup>4</sup>; Oliver Y Wang<sup>2</sup>; Rakhi Pandey<sup>1</sup>; Jennifer E. Van Eyk<sup>1,3</sup>; <sup>1</sup>Cedars-Sinai Medical Center, Los Angeles, CA; <sup>2</sup>Cedars-Sinai Medical Center, Los Angeles; <sup>3</sup>Advanced Clinical BioSystems Research Institute, Cedars-Sinai Medical Center, Los Angeles, CA; <sup>4</sup>Cedars-Sinai Precision Biomarker Labs (PBL), Beverly Hills, CA
- WP 428 **Integration of Skyline and PDV into FragPipe for Advanced Visualization**; Fengchao Yu<sup>1</sup>; Matthew Chambers<sup>2</sup>; Kai Li<sup>1</sup>; Daniel Polasky<sup>1</sup>; Brendan MacLean<sup>2</sup>; Alexey Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, Michigan; <sup>2</sup>University of Washington, Seattle, WA
- WP 429 **A Common Data Analysis Pipeline (CDAP) for Data Independent Acquisition Mass Spectrometry Data**; Aaron Maurais<sup>1</sup>; Michael Riffle<sup>1</sup>; Brian Connolly<sup>2</sup>; Matthew Chambers<sup>1</sup>; Brendan X MacLean<sup>3</sup>; Gennifer E Merrihew<sup>3</sup>; Julia E Robbins<sup>3</sup>; Ratna R Thangudu<sup>4</sup>; Brian C. Searle<sup>5</sup>; Christine C Wu<sup>3</sup>; Paul A Rudnick<sup>6</sup>; Michael J. MacCoss<sup>3</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Washington - Laboratory Medicine and Pathology, Seattle, WA; <sup>3</sup>University of Washington - Genome Sciences, Seattle, WA; <sup>4</sup>ICF International, Reston, VA; <sup>5</sup>Ohio State University, Columbus, OH; <sup>6</sup>Spectragen Informatics, Bainbridge Island, WA
- WP 430 **New Outlier Detection Capabilities and Enhanced Reporting in Panorama and AutoQC**; Josh Eckels<sup>1</sup>; Ankur Juneja<sup>1</sup>; Wendy Innis<sup>1</sup>; Sweta Jewargikar<sup>1</sup>; Vagisha Sharma<sup>2</sup>; Nicholas Shulman<sup>2</sup>; Michael J. MacCoss<sup>2</sup>; Brendan MacLean<sup>2</sup>; <sup>1</sup>LabKey, San Diego, CA; <sup>2</sup>University of Washington, Seattle, WA
- INSTRUMENTATION: MINI/PORTABLE/FIELDABLE MS**  
431-442
- WP 431 **A Gas Assisted Bi-helical Reconfigurable Ion Guide for Ambient Mass Spectrometry**; He Xingliang; Sichuan University, Chengdu, China
- WP 432 **Portable Mass Spectrometer for Bioaerosol Detection**; Vadym Berkout<sup>1</sup>; Stuart Collymore<sup>1</sup>; Scott Ecelberger<sup>1</sup>; Max Cetta<sup>1</sup>; Lara Moore<sup>1</sup>; Michael McLoughlin<sup>1</sup>; Wayne Bryden<sup>1</sup>; <sup>1</sup>Zeteo Tech, Inc., Sykesville, MD
- WP 433 **Development of a portable UPLC Mass Spectrometer**; Chung-Hsuan Chen<sup>1</sup>; Ju Yao Chang<sup>1,2</sup>; chun-jen Hsiao<sup>1</sup>; Jung Lee Lin<sup>1</sup>; <sup>1</sup>Genomic Research Center, Taipei, Taiwan; <sup>2</sup>National Sun Yat-Sen University, Kaohsiung, Taiwan
- WP 434 **Portable Instrumentation for SPME Analysis: Beyond the Laboratory**; Enrico Davoli<sup>1</sup>; Alessia Turina<sup>1</sup>; Stefano Carabellese<sup>1</sup>; Alice Passoni<sup>1</sup>; Vladimir M. Doroshenko<sup>2</sup>; <sup>1</sup>Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy; <sup>2</sup>MassTech Inc., Columbia, MD
- WP 435 **Prototype Development of a Digital Linear Ion Trap based Palmtop Mass Spectrometer**; Saifei CHEN<sup>1</sup>; Yongkai CAI<sup>1</sup>; Lin LIU<sup>1</sup>; Hongbing CHENG<sup>1</sup>; Qiao JIN<sup>1</sup>; Yuanyuan HUANG<sup>1</sup>; Wenjian SUN<sup>1</sup>; <sup>1</sup>Shimadzu Research Laboratory (Shanghai) Co.Ltd., Shanghai, China
- WP 436 **Pollinator Watch: Evaluating Environmental Contamination Through Beehive Air Volatiles with Portable Mass Spectrometric Systems**; Daria Ilić<sup>1</sup>; Boris Brkić<sup>1</sup>; Đorđe Vujić<sup>1</sup>; <sup>1</sup>BioSense Institute, Novi Sad, Serbia
- WP 437 **Adapting a DART-MS seized drug analysis workflow to a field deployable, high-resolution mass spectrometry system**; Elizabeth L. Robinson<sup>1</sup>; Meghan G. Appley<sup>1</sup>; Thomas P. Forbes<sup>1</sup>; Edward Sisco<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD
- WP 438 **An APPI Miniature Mass Spectrometer for Real-Time Analysis of BTEX**; David Lewis<sup>1</sup>; Kevin P. Schultze<sup>2</sup>; Mac Gilliland<sup>1</sup>; <sup>1</sup>Furman University, Greenville, SC; <sup>2</sup>908 Devices Inc., Boston, MA
- WP 439 **MOMA Engineering Test Unit Sample Investigation and Database Generation**; Friso H.w. Van Amerom<sup>1,2</sup>; Xiang Li<sup>1</sup>; Marco E Castillo<sup>1,3</sup>; Ryan M. Danell<sup>1,4</sup>; Desmond A. Kaplan<sup>1,5</sup>; Andrej Grubisic<sup>1</sup>; Teresa Fornaro<sup>6</sup>; William B Brinckerhoff<sup>1</sup>; And The MOMA Team<sup>7</sup>; <sup>1</sup>NASA Goddard Space Flight Center, Greenbelt, MD; <sup>2</sup>Mini-Mass Consulting, Inc, Hyattsville, MD; <sup>3</sup>Aerodyne Industries, Cape Canaveral, FL; <sup>4</sup>Danell Consulting Inc, Winterville, NC; <sup>5</sup>KapScience LLC, Tewksbury, MA; <sup>6</sup>INAF-Astrophysical Observatory of Arcetri, Florence, Italy; <sup>7</sup>Max Planck Institut für Sonnensystemforschung, Goettingen, Germany
- WP 440 **Identification of Two Common Diagnostic Peptide Markers in Urine using a Portable Mass Spectrometer**; Dan Carmany<sup>1</sup>; Krisztian Torma<sup>2</sup>; William Yang Terzian<sup>2</sup>; <sup>1</sup>Self Employed, Las Vegas, NV; <sup>2</sup>BaySpec, Inc, San Jose, CA
- WP 441 **Performance of a planetary science instrument prototype with a dual source linear ion trap integrated to an Orbitrap analyzer**; Adrian Southard<sup>1</sup>; Lucas Taft Andrews<sup>2</sup>; Ryan M. Danell<sup>3,4</sup>; Desmond A. Kaplan<sup>4,5</sup>; Steven Rogacki<sup>6</sup>; Friso H.w. Van Amerom<sup>4,7</sup>; Ricardo Arevalo<sup>2</sup>; Niko Minasola<sup>8</sup>; Wally Rodriguez<sup>8</sup>; Diego Garcia<sup>8</sup>; <sup>1</sup>CRESST-II Univ. of Maryland, CP, and NASA GSFC, Greenbelt, MD; <sup>2</sup>University of Maryland, College Park, College park, MD; <sup>3</sup>Danell Consulting, Inc., Winterville, NC; <sup>4</sup>NASA Goddard Space Flight Center, Greenbelt, MD; <sup>5</sup>KapScience LLC, Tewksbury, MA; <sup>6</sup>University of Michigan Space Physics Research Laboratory, Ann Arbor, MI; <sup>7</sup>Mini-Mass Consulting, Inc, Hyattsville, MD; <sup>8</sup>AMU Engineering Inc, Miami, FL
- WP 442 **Simplified, abbreviated screening and confirmatory analysis of cocaine in urine matrix using BioSPME**; Caleigh R O'Connor<sup>1</sup>; Vladimir M. Doroshenko<sup>1</sup>; Enrico Davoli<sup>2</sup>; Nivedita Bhattacharya<sup>3</sup>; Jayeshkumar Das<sup>1</sup>; Venkat Panchagnula<sup>1</sup>; <sup>1</sup>MassTech Inc., Columbia, MD; <sup>2</sup>Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy; <sup>3</sup>Barefeet Analytics Pvt. Ltd., Pune, India

## WEDNESDAY POSTERS

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- WP 443 **Optimization of the Astral detection system: Enabling high linear dynamic range and single-ion sensitivity for deep proteome coverage;** Christian Hock<sup>1</sup>; Johannes Petzoldt<sup>1</sup>; Philipp Cochems<sup>1</sup>; Immo Colonius<sup>1</sup>; Bernd Hagedorn<sup>1</sup>; Arne Kreuzmann<sup>1</sup>; Daniel Mourad<sup>1</sup>; Maximilian Ochmann<sup>1</sup>; Amelia C. Peterson<sup>1</sup>; Hamish Stewart<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Bremen, Germany
- WP 444 **A Novel Long-Lifetime Ion Detector for GC-TOFMS and GCxGC-TOFMS with Sub-Femtogram Detection Limits;** Matthew Soyk<sup>1</sup>; Semyon Shofman<sup>2</sup>; Amit Weingarten<sup>2</sup>; Viatcheslav Artaev<sup>1</sup>; <sup>1</sup>LECO Corporation, St. Joseph, MI; <sup>2</sup>El Mul Technologies, Rehovot, Israel
- WP 445 **A novel long-life detector for a novel high-speed hybrid nominal mass platform;** Oleg Silivra<sup>1</sup>; Philip M. Remes<sup>1</sup>; Linfan Li<sup>1</sup>; Charles Maxey<sup>1</sup>; Cristina Jacob<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA
- WP 446 **Multiple Ion Charge Extraction for High-Throughput Charge Detection Mass Spectrometry;** Raj Parikh<sup>1</sup>; Benjamin Draper<sup>2</sup>; Martin Jarrold<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>Megadallon Solutions, Bloomington, Indiana
- WP 447 **A Digitally Operated Pre-filter Improves Transmission for Higher Stability Zones Accessed Using a Digital Quadrupole Mass Filter;** Fatima Olayemi Obe<sup>1</sup>; Elizabeth Groetsema<sup>1</sup>; Sumeet Chakravorty<sup>1</sup>; Gordon A Anderson<sup>2</sup>; Adam P. Huntley<sup>1</sup>; Brian H. Clowers<sup>1</sup>; Peter T. A. Reilly<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>GAA Custom Electronics LLC, Kennewick, WA
- WP 448 **Experimental Evaluation of the Higher Order Mathieu Space Stability Zones Using a Digitally Operated Mass Filter;** Sumeet S. Chakravorty<sup>1</sup>; Fatima O. Obe<sup>1</sup>; Elizabeth G. Groetsema<sup>1</sup>; Adam P. Huntley<sup>1</sup>; Gordon A. Anderson<sup>2</sup>; Brian H Clowers<sup>1</sup>; Peter T. A. Reilly<sup>1</sup>; <sup>1</sup>Washington State University Department of Chemistry, Pullman, WA; <sup>2</sup>GAA Custom Electronics LLC, Kennewick, WA
- WP 449 **Characterization of RF Imbalance Influence on Black Holes in a Miniature Linear Ion Trap for Space Flight Applications;** Desmond A. Kaplan<sup>1, 2</sup>; Ryan M. Danell<sup>1, 3</sup>; Ryan Barnhart<sup>4</sup>; Jacob D. Graham<sup>1</sup>; Friso Van Amerom<sup>1, 5</sup>; Marco E. Castillo<sup>1, 6</sup>; William B. Brinckerhoff<sup>1</sup>; Andrej Grubisic<sup>1</sup>; Melissa G Trainer<sup>1</sup>; <sup>1</sup>NASA Goddard Space Flight Center, Greenbelt, MD; <sup>2</sup>KapScience LLC, Tewksbury, MA; <sup>3</sup>Danell Consulting, Inc., Winterville, NC; <sup>4</sup>University of Michigan Space Physics Research Laboratory, Ann Arbor, MI; <sup>5</sup>Mini-Mass Consulting, Inc, Hyattsville, MD; <sup>6</sup>Aerodyne Industries LLC, Cape Canaveral, FL
- WP 450 **Development of a Digital Quadrupole Mass Filter with Improved Isolation Efficiency;** Robert Schrader<sup>1</sup>; Gordon A Anderson<sup>2</sup>; David H Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX; <sup>2</sup>GAA Custom Electronics LLC, Kennewick, WA
- WP 451 **Setting the STORI Straight: Improved CDMS Results Via misSTORI Analysis;** Michael Goodwin<sup>1</sup>; Kyle Patrick Bowen<sup>1</sup>; Dmitry Grinfeld<sup>2</sup>; Ping Yip<sup>1</sup>; Michael W Senko<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany
- WP 452 **Detecting High Energy Ions on a High Voltage LIT-MS with a Curved 45-degree Dynode;** Liam Dugan<sup>1</sup>; Mark E Bier<sup>2</sup>; <sup>1</sup>Carnegie Mellon University, Pittsburgh, PA; <sup>2</sup>Carnegie Mellon University, Pittsburgh, Pennsylvania
- WP 453 **Extending the Linear Range of Capacitive Ultra-Wide-Range Current Amplifiers above Eleven Orders of Magnitude;** Cornelius Wendt<sup>1</sup>; Alexander Bohnhorst<sup>1</sup>; Simon Degen<sup>1</sup>; Ansgar T. Kirk<sup>1</sup>; <sup>1</sup>ACKISION GmbH, Hannover, Germany
- WP 454 **Design and Performance Characterization of the Hardware and Electronics for Pulse Counting Detection with a Linear Ion Trap Mass Spectrometer;** Ryan M. Danell<sup>1, 2</sup>; Andrej Grubisic<sup>1</sup>; Jacob D. Graham<sup>1</sup>; Desmond A. Kaplan<sup>1, 3</sup>; Friso Van Amerom<sup>1, 4</sup>; Marco E. Castillo<sup>1, 5</sup>; David R. Durachka<sup>1</sup>; William B. Brinckerhoff<sup>1</sup>; Melissa G. Trainer<sup>1</sup>; <sup>1</sup>NASA Goddard Space Flight Center, Greenbelt, MD; <sup>2</sup>Danell Consulting, Inc., Winterville, NC; <sup>3</sup>KapScience LLC, Tewksbury, MA; <sup>4</sup>Mini-Mass Consulting, Inc, Hyattsville, MD; <sup>5</sup>Aerodyne Industries LLC, Cape Canaveral, FL
- WP 455 **Characterisation of post translational modifications of proteins with ECD fragmentation on a trapped ion mobility spectrometry (TIMS) equipped FT-ICR;** C Logan Mackay<sup>1</sup>; Anthony J Devlin<sup>1</sup>; Anna Simmonds<sup>1</sup>; Christopher A Wootton<sup>2</sup>; Felicia Green<sup>1</sup>; <sup>1</sup>Rosalind Franklin Institute, Harwell, United Kingdom; <sup>2</sup>Bruker Daltonik GmbH & Co. KG, Bremen, Germany
- WP 456 **Characterization of ScintiFast Scintillators in a Microchannel Plate based TOF Detector;** Joe Czekner<sup>1</sup>; Sasha Kadyshевич<sup>2</sup>; Barak Lavi<sup>2</sup>; Stephen Ritzau<sup>1</sup>; Amit Weingarten<sup>2</sup>; <sup>1</sup>Photonis Scientific, Sturbridge, MA; <sup>2</sup>El-Mul Technologies, Rehovot, Israel
- WP 457 **Practical Quadrupole Theory: Digital Quadrupoles vs. Traditional Sinusoidal Operation;** Randall E Pedder<sup>1</sup>; Luke Metzler<sup>1</sup>; Jacob Pasko<sup>1</sup>; Alex Miscovich<sup>1</sup>; Herb Gass<sup>1</sup>; Gordon Anderson<sup>2</sup>; <sup>1</sup>Ardara Technologies, Ardara, PA; <sup>2</sup>GAA Custom Electronics LLC, Kennewick, WA
- WP 458 **Rapid and Reliable Nitrite Content Analysis in Pharmaceutical Excipients with the ACQUITYTM QDaTM II Mass Detector;** Henry Foddy<sup>1</sup>; Amy Bartlett<sup>1</sup>; Victoria Starkie<sup>1</sup>; Jonathan Pugh<sup>1</sup>; Cristian Cojocariu<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom

### ION MOBILITY: FAIMS/DMS 459-465

- WP 459 **Exploring bacterial virulence factors diversity using Field Asymmetric Ion Mobility Spectrometry (FAIMS) and Kendrick Mass Defect (KMD) Plots;** Abanoub Mikhael<sup>1, 2</sup>; Darryl Hardie<sup>1</sup>; Helena Pětrošová<sup>1, 2</sup>; ROBERT K ERNST<sup>3</sup>; DAVID R GOODLETT<sup>1, 2</sup>; <sup>1</sup>UVic Genome BC Proteomics Centre, Victoria, BC; <sup>2</sup>University of Victoria, Victoria, BC; <sup>3</sup>University of Maryland, Baltimore, Baltimore, MD
- WP 460 **Novel Protein Separations Employing the Second Derivative of High-Field Ion Mobility in a Field Gradient;** Atena Tajaddodi<sup>1</sup>; Hayden A Thurman<sup>1</sup>; Alexandre A Shvartsburg<sup>1</sup>; <sup>1</sup>Wichita State University, Wichita, KS
- WP 461 **Parameter optimization of FAIMS nano-LC-MS/MS methods for improved detection of small protein expression differences on an Orbitrap Exploris 480;** Sam M Williamson<sup>1</sup>; Luc A. Tessier<sup>1</sup>; Tammy-Lynn Tremblay<sup>1</sup>; Tyler M. Renner<sup>1</sup>; Jennifer J. Hill<sup>1</sup>; <sup>1</sup>National Research Council of Canada, Ottawa, ON
- WP 462 **Optimization of LC-FAIMS-MS/MS for in-depth proteome characterization of plasma from cattle;** Gustavo Diaz<sup>1</sup>; Dorathe Lee<sup>1</sup>; Corey D Broeckling<sup>1</sup>; <sup>1</sup>Analytical Resources Core: Bioanalysis and Omics Center, Colorado State University, Fort Collins, CO
- WP 463 **A Sensitive Antibody-free FAIMS-dCV/SRM-MS Method for Targeted Protein Quantification;** Qingqing Shen<sup>1</sup>; Jie Pu<sup>1</sup>; Chao Xue<sup>1</sup>; Ming Zhang<sup>1</sup>; Shihan Huo<sup>1</sup>; Wei-Jun Qian<sup>2</sup>; Cornelia L Boeser<sup>3</sup>; Michael W Belford<sup>3</sup>; Charles Maxey<sup>3</sup>; Neloni R. Wijeratne<sup>3</sup>; Claudia Martins<sup>3</sup>; Scott M Peterman<sup>3</sup>; Wang Cao<sup>4</sup>; Jun Qu<sup>1</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>3</sup>ThermoFisher Scientific, San Jose, CA; <sup>4</sup>University at buffalo, buffalo
- WP 464 **Evaluation of FAIMS Coupled with the Orbitrap Astral Mass Spectrometer for Proteomics;** Li-Yu Chen<sup>1</sup>; Katherine A Overmyer<sup>2, 3, 4</sup>; Pavel Sinitcyn<sup>3</sup>; Scott T Quarmby<sup>2</sup>; Joshua J Coon<sup>1, 2, 3, 4</sup>; <sup>1</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>Morgridge Institute for Research, Madison, WI; <sup>4</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI
- WP 465 **Assessing the reduction of interferences in SWATH data-independent acquisition (DIA) with differential mobility separation (DMS);** Yves Le Blanc<sup>1</sup>; Eva Duchoslav<sup>2</sup>; Lyle Burton<sup>2</sup>; Bradley Schneider<sup>2</sup>; <sup>1</sup>SCIEX, Concord, ON, ON; <sup>2</sup>SCIEX, Concord, ON

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### ION MOBILITY: GENERAL 466-479

- WP 466 **Investigation the Effect of Travelling Wave Profiles in Structure for Lossless Ion Manipulation (SLIM);** Mohsen Latif<sup>1</sup>; Viraj Gandhi<sup>1,2</sup>; Leyan Hua<sup>1</sup>; Carlos Iarriba-andaluz<sup>1</sup>; <sup>1</sup>Mechanical Engineering, IUPUI, Indianapolis, IN; <sup>2</sup>Purdue University, West Lafayette, IN
- WP 467 **IonToolPack: a software suit of AI-powered tools for mass spectrometry;** Aivett Bilbao<sup>1</sup>; Andrea Harrison<sup>1</sup>; Samiha Chabane<sup>1</sup>; Ashfiqur Rahman<sup>1</sup>; Nathalie Munoz<sup>1</sup>; Yuqian Gao<sup>2</sup>; Marija Velickovic<sup>1</sup>; Josie G. Eder<sup>2</sup>; Priscila Lalli<sup>2</sup>; Daniel J. Orton<sup>2</sup>; Chaevien S. Clendinen<sup>1</sup>; Vimal K. Balasubramanian<sup>1</sup>; Arunima Bhattacharjee<sup>1</sup>; Christopher R. Anderton<sup>1</sup>; Sarah M. Williams<sup>1</sup>; Sneha P. Couvillion<sup>2</sup>; Thomas L. Fillmore<sup>1</sup>; Karl K. Weitz<sup>2</sup>; Joonhoon Kim<sup>3</sup>; Young-Mo Kim<sup>2</sup>; Tao Liu<sup>2</sup>; Jennifer E. Kyle<sup>2</sup>; Kyle R. Pomraning<sup>3</sup>; Kristin E. Burnum-Johnson<sup>1</sup>; <sup>1</sup>Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; <sup>3</sup>Energy Processes and Materials Division, Pacific Northwest National Laboratory, Richland, WA
- WP 468 **Dual-Path TW-SLIM for Masked Ion Mobility Spectrometry with Complete Ion Utilization;** Cullen Greer<sup>1</sup>; Brian H. Clowers<sup>1</sup>; <sup>1</sup>Washington State University Department of Chemistry, Pullman, WA
- WP 469 **Lowering the Entry Barrier: A Low-Cost Vacuum Enclosure for Ion Funnel, Ion Guides, and Structures for Lossless Ion Manipulations;** Brian H. Clowers<sup>1</sup>; Nathan W. Buzitis<sup>1</sup>; Gustavo Gallardo<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA
- WP 470 **High-efficiency electron capture dissociation of peptides and proteins after collision-induced unfolding and ion mobility;** Joseph C. Meeuwesen<sup>1</sup>; Ruwan T. Kurulugama<sup>1</sup>; Yury V. Vasilev<sup>1</sup>; Valery G. Voinov<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- WP 471 **Comparison of LC-MS/MS, LC-TIMS-MS/MS, and MALDI TIMS MS/MS Methods for Lipidomics;** Min Liu<sup>1</sup>; Carolina Cruz Cepeda<sup>1</sup>; John M. Koomen<sup>1</sup>; <sup>1</sup>Moffitt Cancer Center, Tampa, FL
- WP 472 **Trends in Transition Metal Binding with Polyproline Using Ion Mobility Mass Spectrometry;** Anthony J. Pestrutto<sup>1</sup>; David Clemmer<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN
- WP 473 **Sub-Nyquist Experimental Timescales Using Compressed Sensing Ion Mobility Mass Spectrometry;** Elvin R. Cabrera<sup>1</sup>; Brian H. Clowers<sup>1</sup>; <sup>1</sup>Washington State University Department of Chemistry, Pullman, WA
- WP 474 **Utilizing High Resolution Ion Mobility Spectrometry-Mass Spectrometry for Opioid Profiling;** Jack P. Ryan<sup>1</sup>; James N. Dodds<sup>1</sup>; Erin S. Baker<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC
- WP 475 **Cross Platform Assessment of Feature Detection Capability as a Function of Measured Resolving Power in Ion Mobility Spectrometry (IMS);** James Dodds<sup>1</sup>; Amie M. Solosky<sup>1</sup>; Jack P. Ryan<sup>1</sup>; Erin S. Baker<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC
- WP 476 **Moving IMS to the next level, New Possibilities with Multilevel SLIM;** Adam P. Huntley<sup>1</sup>; Adam L. Hollerbach<sup>1</sup>; Randolph V. Norheim<sup>1</sup>; Ahmed M. Hamid<sup>1</sup>; Gordon A. Anderson<sup>2</sup>; Sandilya V.B. Garimella<sup>1</sup>; Jon M. Jacobs<sup>1</sup>; Richard D. Smith<sup>1</sup>; Yehia M. Ibrahim<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>GAA Custom Electronics LLC, Kennewick, WA
- WP 477 **Accurate CCS Measurement by Multi-pass Cyclic IMS Enables Confident Glycan Structure Assignment;** Chaoshuang Xia<sup>1</sup>; Elias Mernie<sup>1</sup>; Joseph Zaia<sup>1</sup>; Catherine E. Costello<sup>1</sup>; Cheng Lin<sup>2</sup>; <sup>1</sup>Boston University Chobanian & Avedisian School of Medicine, Boston, MA; <sup>2</sup>Boston University, Boston, MA
- WP 478 **Dendrimers and their application as mass and mobility calibration standards – a case study for reliability and applicability;** Jens Sommertune<sup>1</sup>; Emily R. Sekera<sup>2,3</sup>; Claudia Möckel<sup>4</sup>; Florian Stappert<sup>5</sup>; Cedric Thom<sup>5</sup>; Arpad Somogyi<sup>3</sup>; Bela Paizs<sup>6</sup>; Oliver J. Schmitz<sup>5</sup>; <sup>1</sup>Polymer Factory Sweden, Stockholm, Sweden; <sup>2</sup>St Jude Children's Research Hospital, Memphis, TN; <sup>3</sup>Ohio State University, Columbus, OH; <sup>4</sup>Stockholm University, Stockholm, Sweden; <sup>5</sup>University of Duisburg-Essen, Essen, Germany; <sup>6</sup>Rosalind Franklin Institute, Didcot, United Kingdom
- WP 479 **Solving the "General Elution Problem" in Ion Mobility Spectrometry;** Eric Davis<sup>1</sup>; Tristan Koop<sup>1</sup>; Landon Vyhmeister<sup>1</sup>; Saned Gharari<sup>1</sup>; Julia Fehr<sup>1</sup>; Gavin Valdez<sup>1</sup>; <sup>1</sup>Whitworth University, Spokane, WA

### LC/MS: CHROMATOGRAPHY AND SOFTWARE 480-492

- WP 480 **Accurate mass spectral deconvolution of multiply-charged oligonucleotides using unit resolution single quadrupole LC/MS;** Patrick M. Batoon<sup>1</sup>; Lee Bertram<sup>2</sup>; Yongdong Wang<sup>3</sup>; <sup>1</sup>Agilent Technologies Inc., Santa Clara, CA; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>Cerno Biosciences, Las Vegas, NV
- WP 481 **Rapid QC-MS – Interactive Dashboard for Near Synchronous Mass Spectrometry Data Acquisition Quality Control;** Wasim Sandhu<sup>1</sup>; Ira J. Gray<sup>1</sup>; Sarah Lin<sup>1</sup>; Joshua E. Elias<sup>1</sup>; Brian C. DeFelice<sup>1</sup>; <sup>1</sup>Chan Zuckerberg Biohub, San Francisco, CA
- WP 482 **Evaluation of analytical columns in ADC separation for calculation of drug-to-antibody ratio (DAR);** Kazuko Inoue; Eisai Co., Ltd., Tsukuba, Japan
- WP 483 **Automated Online LC-MS Small Molecule Reaction Monitoring with a Single Quadrupole MS;** Dr. Sebastian T. Weinig-Berger<sup>1</sup>; Russell Burge, PhD<sup>2</sup>; Dr. Edgar Naegele<sup>1</sup>; Dr. Andreas Mielcarek<sup>1</sup>; <sup>1</sup>Agilent Technologies, Waldbronn, Germany; <sup>2</sup>Agilent Technologies Inc., Santa Clara, CA
- WP 484 **A Rational Strategy of Peptide Solubilization for Bottom-up Proteomics Using Hydrophilic Interaction Chromatography;** Eisuke Kanao<sup>1,2</sup>; Koshin Akamatsu<sup>1</sup>; Ayana Tomioka<sup>1</sup>; Yasushi Ishihama<sup>1,2</sup>; <sup>1</sup>Kyoto university, Kyoto, Japan; <sup>2</sup>National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan
- WP 485 **Use of tandem Supercritical Fluid Chromatography (SFC) and High-Resolution Mass Spectrometry for Metabolite Characterisation and Identification;** Oleg Chepelin; Charles River Laboratories, Edinburgh, United Kingdom
- WP 486 **Untargeted analysis of hydrophilic metabolites with an improved LC-MS separation using a pentafluorophenyl-functionalized column, and prediction-based MS/MS spectrum annotation;** Masaru Sato<sup>1</sup>; Kazutaka Ikeda<sup>1</sup>; <sup>1</sup>Kazusa DNA Research Institute, 2-6-7 Kazusakamatari, Kisarazu, Japan
- WP 487 **Versatile use of microfluidic LC columns, optimized configuration for achieving significant increases in proteome coverage at low nanoLC flow rates;** Jeff Op De Beeck<sup>1</sup>; Natalie Van Landuyt<sup>1</sup>; Robert Van Ling<sup>2</sup>; Yuan Lin<sup>3</sup>; Paul Jacobs<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Ghent, Belgium; <sup>2</sup>Thermo Fisher Scientific - Breda, Breda, Netherlands; <sup>3</sup>Thermo Fisher Scientific, Sunnyvale, CA
- WP 488 **Enhanced lipidomics analysis with phenyl-hexyl based RPLC-MS;** Yikun Liu<sup>1</sup>; Jinling Lu<sup>1</sup>; Wenpeng Zhang<sup>1</sup>; Zheng Ouyang<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China
- WP 489 **Vendor-neutral, Browser-Based Advanced MS Data Processing;** Ryan Andrews<sup>1</sup>; Anne Marie Smith<sup>1</sup>; Richard Lee<sup>1</sup>; Sofya Chudova<sup>1</sup>; Vitaly Lashin<sup>1</sup>; Rostislav Pol<sup>1</sup>; <sup>1</sup>ACD/Labs, Toronto, ON
- WP 490 **Method Development of PFAS Compounds Using a Virtual Method Development Tool;** Melinda D. Urlich<sup>1</sup>; Justin Steimling<sup>1</sup>; Chris Nelson<sup>1</sup>; Tim Yosca<sup>1</sup>; John Garrett<sup>2</sup>; Elena Gairloch<sup>1</sup>; <sup>1</sup>Restek Corporation, Bellefonte, PA; <sup>2</sup>Analytical Innovations, Dayton, OH
- WP 491 **Elevating Precision in Single-Cell Applications: A Breakthrough with Monolithic Silica Capillary Columns;** Michael Krawitzky<sup>1,2</sup>; Mario Mirabelli<sup>2</sup>; Florian Busch<sup>2</sup>; Goran Mitulovic<sup>2</sup>; Jean-François Greisch<sup>2</sup>; Gary Kruppa<sup>3</sup>; <sup>1</sup>Bruker Daltonics, San Jose, CA; <sup>2</sup>Bruker Switzerland AG,

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- Faellanden, Switzerland; <sup>3</sup>Bruker S.R.O., Brno, Czech Republic
- WP 492 **On-line HIC-MS for the Analysis of ADCs;** Steven C Pomerantz<sup>1</sup>; Eilyn Lacy<sup>1</sup>; Richard Huang<sup>1</sup>; Steven Jacobs<sup>1</sup>; <sup>1</sup>Janssen Research and Development, Spring House, PA
- LC/MS: SAMPLE PREPARATION II**  
493-512
- WP 493 **Automated Liquid-Liquid Extraction and Determination of Abused OTC Compounds in Serum and Urine Samples using a Robotic Autosampler and LC-MS/MS;** Fred Foster; Gerstel, Inc., Linthicum, MD
- WP 494 **Development of a Portable and Rapid Hydrogel-Based Proteomic Workflow;** Maor Arad<sup>1,2</sup>; Connor Frey<sup>1,2</sup>; Rhien Hare<sup>2,3</sup>; Ronald Balagtas<sup>2</sup>; Dario Jereb<sup>2</sup>; Zach Nestman<sup>2</sup>; Manjot Benning<sup>2</sup>; Kenneth Ku<sup>2</sup>; Osei Fordwour<sup>1</sup>; Golfam Ghafourifar<sup>2</sup>; Leonard J Foster<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, BC; <sup>2</sup>University of the Fraser Valley, Abbotsford, BC; <sup>3</sup>Simon Fraser University, Burnaby, BC
- WP 495 **Sample Preparation and Cleanup of Adeno-Associated Virus 6 (AAV6) Capsid Proteins for LC-MS Characterization;** Sitora Khodjaniyazova<sup>1</sup>; Thomas Raymond Slaney<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb, New Brunswick, NJ
- WP 496 **Quantitative Analysis of Legacy & Emerging PFAS in Semiconductor Lubricant using Triple Quadrupole LC/MS;** Stephan Baumann<sup>1</sup>; Aimei Zou<sup>2</sup>; Clyde Helena<sup>3</sup>; <sup>1</sup>Agilent Technologies Inc., Atlanta, GA; <sup>2</sup>Agilent Technologies Singapore, Singapore, Singapore; <sup>3</sup>ASC group, Bentonville, AR
- WP 497 **Development and optimization of a method for automated peptide desalting on the DigestPro MSI robot using AttractSPE® C18 tips;** Célia Jardin<sup>1</sup>; Soumia Hamada<sup>1</sup>; Cédric Pionneau<sup>1</sup>; Martin Technau<sup>2</sup>; Mana Shafaei<sup>3</sup>; Florine Hallez<sup>4</sup>; Michel Arotçarena<sup>4</sup>; Sami Bayoudh<sup>4</sup>; Kaynoush Naraghi<sup>4</sup>; Solenne Chardonnet<sup>1</sup>; <sup>1</sup>Sorbonne University, Inserm, UMS Production et Analyse des données en Sciences de la vie et en Santé (PASS), Plateforme Post-génomique de la Pitié-Salpêtrière (P3S), Paris, France; <sup>2</sup>CEM GmbH, Kamp-Lintfort, Germany; <sup>3</sup>AFFINISEP USA, Miami, FL; <sup>4</sup>AFFINISEP, Le Houllme, France
- WP 498 **Fast and Efficient LC-MS/MS Analysis of PFAS for Clinical Research Using Microelution SPE;** Shahana Wahab Hug<sup>1</sup>; Galo Orquera-Aguirre<sup>1</sup>; Stephanie J. Marin<sup>1</sup>; <sup>1</sup>Phenomenex, Torrance, CA
- WP 499 **Paving the Fast Lane of Biotherapeutic Discovery: Enhancing Throughput via Pre-Allocated Enzyme-Loaded PNGase F Plates for N-Linked Glycan Removal;** Olivia Huffman; Eli Lilly & Co, San Diego
- WP 500 **Proteonano™: a nanobinder-based deep proteomics platform for complex biofluid sample analysis enabling detection of a wide dynamic range of proteins;** Ziquan Cao<sup>1</sup>; Xiehua Ouyang<sup>1</sup>; Libing Wang<sup>1</sup>; Shanshan Lv<sup>1</sup>; Xin Du<sup>1</sup>; Yanting Meng<sup>1</sup>; Yonghao Zhang<sup>1</sup>; Yi Wang<sup>1</sup>; Jie Jin<sup>2,3</sup>; Yang Li<sup>2,3</sup>; Hao Wu<sup>1</sup>; <sup>1</sup>Nanomics Biotechnology, Hangzhou, China; <sup>2</sup>Wuhan Biorun BioSciences Co.,Ltd, Wuhan, China; <sup>3</sup>Wuhan Institute of Biotechnology, Wuhan, China
- WP 501 **High-throughput and automated cellular and tissue lysis using COVARIS acoustic technology for proteomics;** Josselin Ortiz<sup>1</sup>; Angel Keoseyan<sup>1</sup>; Santosh D Bhosale<sup>1</sup>; Nathan Hendricks<sup>1</sup>; Saeed Seyedmohammad<sup>2</sup>; Sameer Vasantgadkar<sup>3</sup>; Lia Abarzua<sup>3</sup>; Annie Moradian<sup>1</sup>; Susan M. Mockus<sup>1</sup>; Jennifer E. Van Eyk<sup>1,2</sup>; <sup>1</sup>Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA; <sup>2</sup>Smidth Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA; <sup>3</sup>Covaris, LLC, Woburn, MA
- WP 502 **Characterization of the New PAL Micro-SPE Cartridge for Pesticides Extract Clean-up;** Jonathan Beck<sup>1</sup>; Hans-Joachim Huebschmann<sup>2</sup>; Lucas Luethy<sup>2</sup>; <sup>1</sup>CTC Analytics AG, Lake Elmo, MN; <sup>2</sup>CTC Analytics AG, Zwingen, Switzerland
- WP 503 **Automated workflow for antibody production and analysis on a robotic liquid handling platform;** Boren Lin<sup>1</sup>; Rinat R Abzalimov<sup>2</sup>; Kinnari Watson<sup>1</sup>; <sup>1</sup>Opentrons Labworks, New York, NY; <sup>2</sup>Advanced Science Research Center, The City University of New York, New York, New York
- WP 504 **Investigating Greener Alternative Detergents for Application in MS Sample Preparation;** Joanna M Gongora<sup>1</sup>; Francisca N De Luna Vitorino<sup>1</sup>; Benjamin A Garcia<sup>1</sup>; <sup>1</sup>Washington University School of Medicine, St. Louis, MO
- WP 505 **Analysis of 6PPD-Quinone in Salmon: A Simplified Sample Prep;** Tina Chambers<sup>1</sup>; Jennifer Cottine Hitchcock<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- WP 506 **Bioanalytical quantification of a lipid conjugated anti-sense oligonucleotide on a HRMS system;** Nikunj Tanna<sup>1</sup>; Mary Trudeau<sup>1</sup>; Joe Fredette<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- WP 507 **Improved Tissue Homogenization and SPE-Based Sample Preparations for the Quantitative LC-MS analysis of Oligonucleotide Therapeutics;** Makda Araya<sup>1</sup>; Kim Tran<sup>1</sup>; Mary Trudeau<sup>1</sup>; Joe Fredette<sup>1</sup>; Bala Addepalli<sup>1</sup>; Matthew Lauber<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- WP 508 **Formulation-specific consumer products analysis for alleviating ion-suppression in MS;** Hyeonjeon Cha<sup>1</sup>; Tae-Young Kim<sup>1</sup>; <sup>1</sup>School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea
- WP 509 **A new Approach to Optimising the SPE Extraction of Oligonucleotides;** Colin Pipe<sup>1</sup>; David Dunthorne<sup>1</sup>; Tony Edge<sup>1</sup>; Matthew James<sup>1</sup>; Ed Faden<sup>2</sup>; <sup>1</sup>Avantor, Theale, United Kingdom; <sup>2</sup>MAC-MOD, Chadds Ford, PA
- WP 510 **An improved EasyPep sample preparation method for enrichment and quantitation of host cell proteins;** Jae Choi<sup>1</sup>; Cristina C Jacob<sup>2</sup>; Philip Remes<sup>2</sup>; Oleg Silivra<sup>2</sup>; Terry Hicks<sup>3</sup>; Matthew Daniels<sup>3</sup>; Nikki Jarrett<sup>1</sup>; Kay Opperman<sup>1</sup>; Bhavin Patel<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Rockford, IL; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific, St. Louis, MO
- WP 511 **Mitigating Cross-Contamination of Methamphetamine in Urine During Supported Liquid Extraction;** Alicia Robinson<sup>1</sup>; Yuping Wang<sup>1</sup>; Lamvien Nguyen<sup>1</sup>; James LaPalme<sup>1</sup>; Elizabeth Bair<sup>1</sup>; Ona Adair<sup>1</sup>; <sup>1</sup>SC PHL, Columbia, SC
- WP 512 **High-pH reversed-phase peptide fractionation on innovative SPE microelution well plates for high-throughput and automated workflows in proteomic studies;** Kaynoush Naraghi<sup>1</sup>; Mana Shafaei<sup>2</sup>; Florine Hallez<sup>1</sup>; Michel Arotçarena<sup>1</sup>; Sami Bayoudh<sup>1</sup>; Cerina Chuon<sup>3</sup>; Chiara Guerrero<sup>3</sup>; <sup>1</sup>AFFINISEP, Le Houllme, France; <sup>2</sup>AFFINISEP USA, Miami, FL; <sup>3</sup>INSERM – US24 SFR Necker Proteome, Paris, France
- METABOLOMICS: TARGETED AND QUANTITATIVE ANALYSIS**  
513-533
- WP 513 **High Throughput Targeted Metabolomics Library Generation on a Novel Mass Spectrometer Applied to Microbiome Analysis;** Bashar Amer<sup>1</sup>; Cristina Jacob<sup>1</sup>; Rahul Deshpande<sup>1</sup>; Reza Jafari<sup>2</sup>; Thomas Moehring<sup>3</sup>; Susan S Bird<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>MetaSci, Toronto, Ontario; <sup>3</sup>Thermo Fisher Scientific, Bremen, Germany
- WP 514 **A combined targeted-untargeted metabolomics workflow for the identification and quantitation of metabolites in complex matrices;** Paul RS Baker<sup>1</sup>; Rebekah Sayers<sup>2</sup>; Cagakan Ozbalci<sup>2</sup>; Robert Proos<sup>1</sup>; <sup>1</sup>SCIEX, USA, Framingham, MASSACHUSETTS; <sup>2</sup>SCIEX UK, Macclesfield, United Kingdom
- WP 515 **An improvised method for simplified simultaneous quantitation of the constituents of a chemically complex mixture;** Chris Beecher<sup>1</sup>; Vladimir Shulaev<sup>2</sup>; Debasish Ghosh<sup>2</sup>; Felice de Jong<sup>1</sup>; Alexander Raskind<sup>1</sup>; <sup>1</sup>IROA Technologies LLC, Nellysford, VA; <sup>2</sup>UNIVERSITY OF NORTH TEXAS, Denton, TX
- WP 516 **Widely targeted volatilities and volatile-GWAS based aromatic rice breeding;** Jie Luo; Hainan University, Sanya, China

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- WP 517 **Quantification of TCA cycle metabolites with automated sample prep, reproducible HILIC chromatography and ion funnel triple quadrupole;** Bianca Ferreira da Silva<sup>1</sup>; Cate Simmermaker<sup>2</sup>; Sierra D. Durham<sup>2</sup>; Karen E. Yannell<sup>2</sup>; <sup>1</sup>Agilent Technologies, Lexington, MA; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- WP 518 **Metabolomic Characterization of a Perfusion Bioprocess System using Pyxis – A Machine Learning Tool for Absolute Quantitation;** Erin Weisenhorn<sup>1</sup>; Luke S. Ferro<sup>2</sup>; Jack Howland<sup>2</sup>; Jonathan Mene<sup>1</sup>; Rosemichelle Marzan<sup>1</sup>; Matthew Stebbins<sup>1</sup>; Eric Rynes<sup>1</sup>; Timothy Kassis<sup>2</sup>; Ana S.H. Costa<sup>2</sup>; Jefferson G. Pruyne<sup>2</sup>; Devesh Shah<sup>2</sup>; Joshua D. Lauterbach<sup>2</sup>; Tian Cai<sup>2</sup>; Jennifer M Campbell<sup>2</sup>; Geoffrey Horner<sup>1</sup>; <sup>1</sup>Just - Evotec Biologics, Seattle, WA; <sup>2</sup>Matterworks, Somerville, MA
- WP 519 **Comprehensive analysis of the NAD<sup>+</sup> metabolome in human serum;** Helena Li<sup>1,2</sup>; Junfang Zhao<sup>2</sup>; Siara Michels<sup>1,2</sup>; Kenneth D.R. Setchell<sup>2</sup>; Lindsey Romick<sup>2</sup>; Xueheng Zhao<sup>2</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH; <sup>2</sup>Division of Pathology & Laboratory Medicine, Cincinnati Children's Hospital Medical Center, Cincinnati, OH
- WP 520 **Correlation of soluble metabolites with Lactate Switch Observed in HEK293 Culture using Novel CE-MS Metabolomics Workflow;** Catherine Rawlins<sup>1</sup>; Erin Redman<sup>2</sup>; Milla Neffling<sup>1</sup>; Stephanie Klaubert<sup>1</sup>; Awab Nehala<sup>1</sup>; J. Will Thompson<sup>2</sup>; <sup>1</sup>908 Devices Inc., Boston, MA; <sup>2</sup>908 Devices Inc., Morrisville, NC
- WP 521 **MASS SPECTROMETRY BASED NUTRIMETABOLOMICS AS A POWERFUL PLATFORM FOR MILLETS;** Sugasini Dhavamani<sup>1</sup>; Anchal Sharma<sup>2</sup>; Prasanth Kumar Punathil Kannan<sup>3</sup>; Raja Lakshitha<sup>4</sup>; Vidya Gundlapalli<sup>5</sup>; Nicole Lysik<sup>6</sup>; Sutape Chantapim<sup>6,7</sup>; <sup>1</sup>Department of Medicine, University of Illinois at Chicago, Chicago, IL; <sup>2</sup>Department of Chemistry, Research Core Facility, University of Illinois at Chicago, Chicago, IL; <sup>3</sup>Department of Pediatrics, University of Illinois at Chicago, Chicago, IL; <sup>4</sup>Tamilnadu Agricultural University, Madurai, India; <sup>5</sup>Department of Chemistry, Loyola University, Chicago, IL; <sup>6</sup>Department of Medicine, University of Illinois Chicago, Chicago, IL; <sup>7</sup>University of Illinois at Chicago, Chicago, IL
- WP 522 **NADomic LCMS separating isobaric and close-mass metabolites in both salvage and kynurenine pathways;** Rong Meng<sup>1</sup>; Katharine D'Aquino<sup>1</sup>; Jose Antonio Chavez<sup>1,2</sup>; Annette Eckardt<sup>1</sup>; Tobias Schips<sup>1</sup>; Karl Kavalkovich<sup>1</sup>; Simon Hinke<sup>1</sup>; Andrea Nawrocki<sup>1</sup>; <sup>1</sup>Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania; <sup>2</sup>Quotient Therapeutics, Cambridge, MASSACHUSETTS
- WP 523 **Simultaneous consideration of within-injection and cross-injection aggregated EIC properties for improved quantitation in LC-MS MRM metabolomics datasets;** Phillip Seitzer<sup>1</sup>; Alireza Delfarah<sup>1</sup>; Johanna Fleischman<sup>1</sup>; Edward S Folk<sup>1</sup>; Celeste Sandoval<sup>1</sup>; Ngoc Vu<sup>1</sup>; Bryson Bennett<sup>1</sup>; <sup>1</sup>Calico Life Sciences, LLC, South San Francisco, CA
- WP 524 **A high-sensitivity UPLC-MRM/MS method for metabolomic analysis of isoprenoid lipids;** Jun Han<sup>1,2</sup>; Juncong Yang<sup>1</sup>; Katelyn McMurray<sup>1</sup>; Malia Lampard<sup>1</sup>; Dave Schibli<sup>1,2</sup>; David R Goodlett<sup>1,3</sup>; <sup>1</sup>Genome BC Proteomics Centre, University of Victoria, Victoria, BC; <sup>2</sup>Division of Medical Sciences, University of Victoria, Victoria, BC; <sup>3</sup>Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC
- WP 525 **Validation of Targeted Quantitative Analysis of Endogenous Biomarkers for Good Clinical Practice Studies;** Maggie Rossow<sup>1</sup>; Lisa Ford<sup>1</sup>; Deirdre Hauser<sup>1</sup>; Anne M Evans<sup>1</sup>; <sup>1</sup>Metabolon Inc., Morrisville, NC
- WP 526 **A novel ML approach to rapidly analyze changes in metabolite concentrations in algae fermentation for bioprocess optimization;** Jack Howland<sup>1</sup>; Frank Xu<sup>2</sup>; Bokkyoo Jun<sup>2</sup>; Yao Lu<sup>2</sup>; Lisa Laprade<sup>2</sup>; Travis Korosh<sup>2</sup>; Luke S Ferro<sup>1</sup>; Ana S.H. Costa<sup>1</sup>; Joshua D. Lauterbach<sup>1</sup>; Jefferson G. Pruyne<sup>1</sup>; Devesh Shah<sup>1</sup>; Timothy Kassis<sup>1</sup>; Jennifer M Campbell<sup>1</sup>; <sup>1</sup>Matterworks, Inc., Somerville, MA; <sup>2</sup>DSM North America, Columbia, MD
- WP 527 **Evaluating a Novel Microchip CE Platform for Use in High-Throughput Quantitative Metabolomics;** Cristina Di Poto<sup>1</sup>; Xiang Tian<sup>1</sup>; Hampus Engstroem<sup>2</sup>; Erin A. Redman<sup>2</sup>; J. Scott Mellors<sup>2</sup>; J. Will Thompson<sup>2</sup>; Sonja Hess<sup>1</sup>; Erik L. Allman<sup>1</sup>; <sup>1</sup>Dynamic Omics, Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD; <sup>2</sup>908 Devices Inc., Morrisville, NC
- WP 528 **Targeted Desorption Electrospray Ionization Mass Spectrometry Imaging For Central Carbon Metabolite Distribution In Mouse Tissue Samples;** Virag Sagi-Kiss<sup>1</sup>; Yayue Song<sup>2</sup>; Brittannie Willis<sup>1,2</sup>; Daniel Simon<sup>1,3</sup>; Duncan Connor Roberts<sup>1</sup>; Suqian Zhang<sup>2</sup>; Simone Di Giovanni<sup>2</sup>; Harry J Whitwell<sup>1</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Department of Metabolism, Digestion and Reproduction; Imperial College London, London, United Kingdom; <sup>2</sup>Division of Neuroscience, Department of Brain Sciences, Imperial College London, London, United Kingdom; <sup>3</sup>Rosalind Franklin Institute, Harwell, United Kingdom
- WP 529 **Disrupted Lipid Metabolism and Cardiomyopathy: Unraveling the Impact of Mitochondrial Fission Factor Loss through Multi-Organ Targeted Metabolomics;** Prasanna Vadhana Ashok Kumar<sup>1</sup>; Olga Bielska<sup>1</sup>; Wendy Jara<sup>1</sup>; Anne Marker<sup>1</sup>; Birgit Schilling<sup>1</sup>; Eric Verdin<sup>1</sup>; <sup>1</sup>Buck Institute for Research on Aging, Novato, CA
- WP 530 **From structure to signal: prediction of molecular response rates in mass spectrometry from 3D conformations;** Yuhui Hong<sup>1</sup>; Chhavi Thakur<sup>1</sup>; Sujun Li<sup>1,2</sup>; Christopher J Welch<sup>3</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>Indiana University Bloomington, Bloomington, IN; <sup>2</sup>GlycoMS LLC, Bloomington, IN; <sup>3</sup>Indiana Consortium for Analytical Science & Engineering (ICASE), Indianapolis, IN
- WP 531 **Targeted Metabolic Profiling of Tryptophan, Tyrosine and Branched Chain Amino Acid Metabolism;** Vladimir Shulaev<sup>1</sup>; Debasish Ghosh<sup>1</sup>; Geoff Faden<sup>2</sup>; Ed Faden<sup>2</sup>; <sup>1</sup>University of North Texas, Denton, TX; <sup>2</sup>MAC-MOD Analytical, Chadds Ford, PA
- WP 532 **Influence of sex and high-fat diet on the regional heterogeneity of bile acid profiles in the intestine of C57BL/6 mice;** Yan Ni<sup>1</sup>; Chuanhao Yang<sup>1,2</sup>; Ana Liu<sup>1</sup>; Huiying Wang<sup>1</sup>; Hongtao Liu<sup>1,2</sup>; Cuifang Xu<sup>1</sup>; Rong Rong<sup>2</sup>; Qingtao Lv<sup>2</sup>; <sup>1</sup>Children's Hospital, Zhejiang University School of Medicine, National Clinical Research Center for Child Health, Hangzhou, China; <sup>2</sup>Shandong University of Traditional Chinese Medicine, Jinan, China
- WP 533 **Method development for quantitatively measuring sex steroids in plasma or serum;** Linxing Yao<sup>1</sup>; Corey Broeckling<sup>1</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO

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- WP 534 **Multimodal analysis of neurodegeneration related changes in lipidomic profiles as a function of diet;** Catelynn C Shafer<sup>1</sup>; Jacopo Di Lucente<sup>1</sup>; Izumi Maezawa<sup>1</sup>; Lee-Way Jin<sup>1</sup>; Elizabeth K Neumann<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA
- WP 535 **Characterization of brain  $\alpha$ -synuclein in neurodegenerative diseases by high-resolution mass spectrometry;** Kim-Thanh VAN<sup>1</sup>; Nicolas Villain<sup>2</sup>; Foudil Lamari<sup>2</sup>; Susana Casas BOLUDA<sup>2</sup>; François Fenaille<sup>1</sup>; François Becher<sup>1</sup>; <sup>1</sup>CEA Paris-Saclay, Gif sur Yvette, France; <sup>2</sup>Hôpitaux Universitaires Pitié Salpêtrière, Paris, France
- WP 536 **A silicon nanodialysis probe coupled with ZipChip CE-MS enables localized in vivo sampling for monitoring brain chemistry;** Kevin Li<sup>1</sup>; Weihua Shi<sup>1</sup>; Yu Ding<sup>1</sup>; Alex George Armstrong<sup>1</sup>; Stanislav Rubakhin<sup>1</sup>; Yurii A Vlasov<sup>1</sup>; Jonathan V Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois-Urbana Champaign, Urbana, IL
- WP 537 **In-depth proteome profiling of the hippocampus of Ldlr knockout mice reveals alternation in the synaptic signaling pathway;** Hong-Beom Park<sup>1,2,3</sup>; Hoesek Seo<sup>2,3,4</sup>;

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- Eunji Jeon<sup>2, 3</sup>; Gyuri Park<sup>3, 5</sup>; Hyeon Chang Lee<sup>3, 5</sup>; Jayun Choi<sup>3, 6</sup>; Sinae Lee<sup>3, 6</sup>; Dohyun Han<sup>2, 3</sup>; <sup>1</sup>Department of Biomedical Science, College of Medicine, Seoul National University, Seoul, South Korea; <sup>2</sup>Department of transdisciplinary medicine, Seoul National University Hospital, Seoul, South Korea; <sup>3</sup>Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; <sup>4</sup>Interdisciplinary Program in Neuroscience, College of Natural Sciences, Seoul National University, Seoul, South Korea; <sup>5</sup>Molecular Medicine and Biopharmaceutical Sciences, WCU Graduate School of Convergence Science and Technology Seoul National University, Seoul, South Korea; <sup>6</sup>Cancer Research institute, Seoul National University college of medicine, Seoul, South Korea
- WP 538 **Multi-omics Evaluation of Human iPSCs and iPSC-derived Neurons**; Gwangbin Lee<sup>1</sup>; Wan Nur Atiqah Binti Mazli<sup>1</sup>; Ling Hao<sup>1</sup>; <sup>1</sup>Department of Chemistry, George Washington University, Washington, DC, United States, Washington, D.C., DC
- WP 539 **CEREBROSPINAL FLUID APOE GLYCOSYLATION ASSOCIATES WITH BIOMARKERS OF ALZHEIMER'S DISEASE PATHOLOGY**; Dobrin Nedelkov<sup>1</sup>; Zoe Tsokolas<sup>2</sup>; Isabel Sible<sup>2</sup>; Wendy J Mack<sup>2</sup>; S Duke Han<sup>2</sup>; John SC Rodman<sup>2</sup>; Hussein N Yassine<sup>2</sup>; <sup>1</sup>Isoformix, Sugar Land, TX; <sup>2</sup>University of Southern California, Los Angeles, CA
- WP 540 **Proteomic analysis on Postmortem Brain Tissue for Molecular Characterization of Chronic Neurodegenerative Diseases Induced by Traumatic Brain Injury**; Junho Park<sup>1, 2</sup>; Dongyoon Shin<sup>2</sup>; Dohyun Han<sup>3</sup>; Yeongshin Kim<sup>5</sup>; Hoon Ryu<sup>6, 7, 8</sup>; Youngsoo Kim<sup>2, 5</sup>; <sup>1</sup>Department of Pharmacology, CHA University School of Medicine, Seongnam-si, South Korea; <sup>2</sup>Proteomics Research Team, CHA Future Medicine Research Institute, Seongnam-si, South Korea; <sup>3</sup>Proteomics Core Facility, Biomedical Research Institute, Seoul, South Korea; <sup>4</sup>Transdisciplinary Department of Medicine & Advanced Technology, Seoul National University Hospital, Seoul, South Korea; <sup>5</sup>Department of Medical Science, CHA University School of Medicine, Seongnam-si, South Korea; <sup>6</sup>Boston University Alzheimer's Disease Center, Boston, MA; <sup>7</sup>Department of Neurology, Boston University School of Medicine, Boston, MA; <sup>8</sup>Brain Science Institute, Korea Institute of Science and Technology (KIST), Seoul, South Korea
- WP 541 **Analysis of Age- and Sex-Related Protein Stability Changes Brain Tissue Cell Lysates from a Mouse Model of Alzheimer's Disease**; Yun Tang<sup>1</sup>; Michael C. Fitzgerald<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC
- WP 542 **Development of a rapid LC-MS/MS method for determination of 13 organophosphorus pesticides and metabolites in human serum**; Maya Rae N Mugosa<sup>1</sup>; Tammy Jones-Lepp<sup>1</sup>; Erin N Toledano Strom<sup>1</sup>; Ruth Marfil-Vega<sup>2</sup>; Celica Cosme<sup>3</sup>; Loren Gabriel Pasia<sup>1</sup>; Justin Miller<sup>4</sup>; Aaron Ritter<sup>4</sup>; Jefferson W Kinney<sup>1</sup>; Stephen Kurzyniec<sup>2</sup>; <sup>1</sup>Pam Quirk Brain Health and Biomarker Laboratory, Department of Brain Health, School of Integrated Health Sciences, University of Nevada Las Vegas, Las Vegas, Nevada; <sup>2</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>3</sup>University of Nevada Las Vegas, Kirk Kerkorian School of Medicine, Las Vegas, Nevada; <sup>4</sup>Cleveland Clinic Lou Ruvo Center for Brain Health, Las Vegas, Nevada
- WP 543 **Differential proteomics in enteroendocrine cells to investigate a brain axis model of Parkinson's disease**; Ying Yan<sup>1</sup>; Julia Balsamo<sup>2</sup>; Elizabeth N Bess<sup>2</sup>; Stephanie M Cologna<sup>1</sup>; <sup>1</sup>University of Illinois Chicago, Chicago, IL; <sup>2</sup>University of California, Irvine, Irvine, CA
- WP 544 **Brain glycoproteomics and proteomics analyses reveal key glycosylated lysine residues of hallmark proteins pathologically associated with Alzheimer's disease**; Qin Fu<sup>1</sup>; Elizabeth T. Anderson<sup>1</sup>; Gary E. Gibson<sup>2</sup>; Sarah A. Flowers<sup>3</sup>; Sheng Zhang<sup>1</sup>; <sup>1</sup>Proteomics and Metabolomics Facility, Cornell University, Ithaca, NY; <sup>2</sup>Weill Cornell Medicine, Burke Neurological Institute, White Plains, NY; <sup>3</sup>Department of Neuroscience, University of Virginia, Charlottesville, VA
- WP 545 **Characterizing Amyloidogenic Protein Oligomers by Native and Top-Down Mass Spectrometry**; Eileen Jacqueline Olivares<sup>1</sup>; Carter Lantz<sup>2</sup>; Rachel Loo<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>University of California, Los Angeles, Los Angeles, CA; <sup>2</sup>Texas A&M University, College Station, TX
- WP 546 **Mapping the human hippocampus using spatial tissue proteomics**; Johanna Tüshaus<sup>1</sup>; Lisa Abel<sup>2</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>TU Munich, Freising, Germany; <sup>2</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- WP 547 **Molecular spatial distribution in transgenic rat model of Alzheimer's disease using MALDI MS imaging**; Tong Shen<sup>1</sup>; Pamela Lein<sup>2</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>West Coast Metabolomics Center, University of California, Davis, Davis, CA; <sup>2</sup>Department of Molecular Biosciences, School of Veterinary Medicine, University of California, Davis, Davis, CA
- WP 548 **Risk assessment for dementia and Alzheimer's disease using plasma amyloid biomarker quantification by immunoprecipitation-mass spectrometry**; Jana Kindermans<sup>1</sup>; Germain Ulysse Busto<sup>2, 3</sup>; Christophe Hirtz<sup>1</sup>; Isabelle Carriere<sup>2</sup>; Karim Bennys<sup>2, 3</sup>; Laure-Anne Gutierrez<sup>2</sup>; Catherine Helmer<sup>4</sup>; Audrey Gabelle<sup>2, 3</sup>; Claudine Berr<sup>2</sup>; Sylvain Lehmann<sup>1</sup>; <sup>1</sup>LBPC-PPC, Montpellier University, IRMB CHU Montpellier, INM INSERM, Montpellier, France; <sup>2</sup>INM, University of Montpellier, INSERM, Montpellier, France; <sup>3</sup>Memory Resource and Research Center, Department of Neurology, University of Montpellier Hospital, Montpellier, France; <sup>4</sup>University of Bordeaux, INSERM UMR U1219, Bordeaux Population Health (BPH) Research Centre, BORDEAUX, France
- WP 549 **Proteomic signatures of sex and social environment: a comparative analysis of the midbrain periaqueductal gray, hippocampus, and cortex**; Kristina Desch<sup>1, 2</sup>; Elena Kutsarova<sup>1</sup>; Petros Chalas<sup>1</sup>; Imke Wüllenweber<sup>2</sup>; Genesis Rosiles<sup>1</sup>; Vanessa Stempel<sup>1</sup>; Julian D. Langer<sup>1, 2</sup>; <sup>1</sup>Max-Planck-Institute for Brain Research, Frankfurt am Main, Germany; <sup>2</sup>Max-Planck-Institute of Biophysics, Frankfurt am Main, Germany
- WP 550 **Profiling CDKL5-Dependent Phosphoproteome Landscape of Mouse Synaptosome and Hippocampus by DIA Mass Spectrometry**; Yi-Kai Liu<sup>1</sup>; Dayne Martinez<sup>2</sup>; Marco Hadisurya<sup>1</sup>; Zhaolan Zhou<sup>2</sup>; W. Andy Tao<sup>1, 3, 4</sup>; <sup>1</sup>Department of Biochemistry, Purdue University, West Lafayette, IN; <sup>2</sup>Department of Genetics, University of Pennsylvania, Philadelphia, PA; <sup>3</sup>Department of Chemistry, Purdue University, West Lafayette, IN; <sup>4</sup>Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN
- WP 551 **Applications of orthogonal label-free single-shot DIA platforms in understanding pathway heterogeneities in C9orf72 ALS using patient-derived astrocytes and microglia**; Mahmud Hossain<sup>1</sup>; Jaunetta Hill<sup>1</sup>; Steven Rodriguez<sup>1</sup>; Leonardo Rodriguez<sup>1</sup>; James Dodge<sup>1</sup>; Bailin Zhang<sup>1</sup>; Dhiman Ghosh<sup>1</sup>; <sup>1</sup>Sanofi, Cambridge, MA
- WP 552 **Advances in Matrix-assisted Laser Desorption/Ionization-Imaging Mass Spectrometry Capture Chondroitin Sulfate-driven Manipulation of Perineuronal Nets with Implications for Alzheimer's Disease**; Cristiana J Meuret<sup>1</sup>; James Movius<sup>1</sup>; Aaron Hendrickson<sup>1</sup>; Asmit Kumar<sup>2</sup>; Ingrid Redford<sup>1</sup>; Jaden Le<sup>1</sup>; Jarrad Scarlett<sup>1</sup>; Kimberly Alonge<sup>1</sup>; Miklos Guttman<sup>3</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Washington, Seattle; <sup>3</sup>University of Washington, Seattle, WA
- WP 553 **Case study emphasizing the need for proteomics in clinical genetics: RNA-protein discordance in rare neurodegeneration-associated variant of the RNA exosome**; H.R. Sagara Wijeratne<sup>1</sup>; Avery M Runnebohm<sup>1</sup>; Whitney Smith-Kinnaman<sup>1</sup>; Emma H Doud<sup>1</sup>; Stephane Pelletier<sup>1</sup>; Amber L Mosley<sup>1</sup>; <sup>1</sup>Indiana University School of Medicine, Indianapolis, IN

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- WP 554 **An atlas of Histone H3.2 and H4 Proteoform of the Mouse Brain;** Meggie N. Young<sup>1</sup>; Bethany Taylor<sup>2</sup>; Tao Wang<sup>3</sup>; Laura Lavery<sup>4</sup>; Huda Zoghbi<sup>2</sup>; Nicolas L. Young<sup>2</sup>; <sup>1</sup>Baylor College of Medicine, Houston, TX; <sup>2</sup>Baylor College of Medicine, Houston, Texas; <sup>3</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>4</sup>Rice University, Houston, TX
- WP 555 **Quantitative proteomics of white matter brain tissue for the analysis of Alzheimer's disease;** Gennifer E Merrihew<sup>1</sup>; Aaron J. Maurais<sup>1</sup>; Jea Park<sup>1</sup>; Deanna Plubell<sup>1</sup>; Bo Wen<sup>1</sup>; William S Noble<sup>1</sup>; C Dirk Keene<sup>2</sup>; Thomas Montine<sup>3</sup>; Michael J. MacCoss<sup>1</sup>; <sup>1</sup>University of Washington - Genome Sciences, Seattle, WA; <sup>2</sup>University of Washington - Laboratory Medicine and Pathology, Seattle, WA; <sup>3</sup>Stanford University - Pathology, Stanford, CA
- WP 556 **Sex-specific Differences in Distributions of Small Molecules in Brain Regions of Alzheimer's Disease Mouse Model using DESI-MSI;** BEHNAZ AKBARI<sup>1</sup>; Victoria L. Wendt<sup>1</sup>; Jitika Rajpoot<sup>2</sup>; Christina R. Ferreira<sup>3</sup>; Caitlin Randolph<sup>2</sup>; Connor H Beveridge<sup>2</sup>; Aditya Kangune<sup>4</sup>; Palak Manchanda<sup>1</sup>; Gaurav Chopra<sup>2</sup>; <sup>1</sup>Purdue University, Department of Chemistry, West Lafayette, IN; <sup>2</sup>Purdue University Department of Chemistry, West Lafayette, IN; <sup>3</sup>Bindley Bioscience Center, Purdue University, West Lafayette, Indiana; <sup>4</sup>Purdue University, Department of Statistics, West Lafayette, IN
- WP 557 **Linking Soil Chemistry to Parkinson's Disease Pathogenesis: Novel Neurodegenerative Compounds from *Streptomyces venezuelae*;** Timothy J Bushman<sup>1</sup>; Osagie Emokpae<sup>1</sup>; Jennifer L Thies<sup>1</sup>; Lena Seyfarth<sup>1</sup>; Elizabeth Gokie<sup>1</sup>; Brandon J Kim<sup>1</sup>; Kim A Caldwell<sup>1</sup>; Lukasz Ciesla<sup>1</sup>; <sup>1</sup>The University of Alabama, Tuscaloosa, AL
- WP 558 **Can Unique Biomarkers Be Identified for 'Exophers'? - An LCM-MS Study;** Megan Hong<sup>1</sup>; Rachel Loo<sup>1</sup>; Joseph Loo<sup>1</sup>; Gal Bitan<sup>1</sup>; Prashant Kaushal<sup>1</sup>; Mehdi Bouhaddou<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles, CA
- NUCLEIC ACIDS AND OLIGONUCLEOTIDES III**  
**559-585**
- WP 559 **Analysis of Posttranscriptional RNA Modifications with MetaMorpheus;** Isabella T Whitworth<sup>1</sup>; Nicholas E Bollis<sup>1</sup>; Mark Scaff<sup>1</sup>; Michael R Shortreed<sup>1</sup>; Lloyd M Smith<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI
- WP 560 **Developing LC-MS based Methods for Routine Quality Control Testing of Phosphoramidite Starting Materials for Oligonucleotide Therapeutics;** Rajeswari Lakshmanan<sup>1</sup>; Steve Rice<sup>1</sup>; Phil Olsen<sup>1</sup>; Dennis Rhodes<sup>1</sup>; Claus Rentel<sup>1</sup>; <sup>1</sup>Ionis Pharmaceuticals, Inc., Carlsbad, CA
- WP 561 **Sequencing of Phosphorodiamidate Morpholino Oligomers by Hydrophilic Interaction Chromatography Coupled to Tandem Mass Spectrometry;** Mingming Wang<sup>1</sup>; Brian O'Day<sup>1</sup>; Brian Michaels<sup>1</sup>; Tao Wei<sup>1</sup>; Jurjus Jurayj<sup>1</sup>; Bao Zhong Cai<sup>1</sup>; <sup>1</sup>Sarepta Therapeutics, Andover, MA
- WP 562 **Assessment of assay-related overdigestion in mRNA poly(A) analysis by LC-MS;** James Boslett<sup>1</sup>; Hannah Demirovic<sup>2</sup>; Janice Wei<sup>1</sup>; Miraslava Potapenko<sup>1</sup>; Oleg Jouravlev<sup>1</sup>; Fanyu Meng<sup>1</sup>; <sup>1</sup>Pfizer, Pearl River, NY; <sup>2</sup>Stony Brook University, Stony Brook, NY
- WP 563 **Mapping tRNA Modifications of *Spinacia oleracea* Using LC-MS/MS;** Bibek Hamal<sup>1</sup>; Patrick A Limbach<sup>1</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH
- WP 564 **Neutral loss scan based LC-MS/MS method for the discovery and characterization of photo-oxidative degradation products of post-transcriptional modified tRNA nucleosides;** Tulsi Bhandari<sup>1</sup>; Balasubrahmanyam Addepalli<sup>2,3</sup>; Patrick A. Limbach<sup>2</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH; <sup>2</sup>University of Cincinnati, Cincinnati, OH; <sup>3</sup>Waters Corporation, Milford, MA
- WP 565 **Nucleoside modification mapping by genome-independent universal mass exclusion list of unmodified oligonucleotides during LC-MS/MS;** Asif Rayhan<sup>1</sup>; Balasubrahmanyam Addepalli<sup>2</sup>; Patrick A. Limbach<sup>2</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH; <sup>2</sup>University of Cincinnati, Cincinnati, OH
- WP 566 **The Addition of Transcriptomics to the Bead-enabled Accelerated Monophasic Multi-omics Method: A Step Toward Universal Sample Preparation;** Joshua D. Breidenbach<sup>1,2</sup>; Emilio S. Rivera<sup>1,2</sup>; Tara Harvey<sup>1,2</sup>; Abigale S. Mikolitis<sup>1,2</sup>; Chi-Yen Tseng<sup>1,2</sup>; Claire K. Sanders<sup>3</sup>; Emilia A. Solomon<sup>2</sup>; Cheryl D. Gleasner<sup>4</sup>; Grace M. Thornhill<sup>1,2</sup>; Kes A. Luchini<sup>1,2</sup>; Brett R. Blackwell<sup>1,2</sup>; Erick S. LeBrun<sup>1,2</sup>; Phillip M. Mach<sup>1,2</sup>; Jennifer F. Harris<sup>5</sup>; Jurgen G. Schmidt<sup>1,2</sup>; Austin R. Anderson<sup>1,2</sup>; Lauren K. Heine<sup>1,2</sup>; Jessica A. Salguero<sup>1,2</sup>; Salvador J. Palmisano<sup>1,2</sup>; Francisca E. Rodriguez<sup>1,2</sup>; Zachary J. Sasiene<sup>1,2</sup>; Ethan M. McBride<sup>1,2</sup>; Trevor G. Glaros<sup>1,2</sup>; <sup>1</sup>Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>3</sup>Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>4</sup>Genomics and Bioanalytics Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>5</sup>Physical Chemistry and Applied Spectroscopy Group, Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM
- WP 567 **Development of a streamlined LC-HRMS/MS-based workflow for identification of mRNA sequence;** Camila A Ortega Ramirez<sup>1</sup>; Julio Hernandez Lopez<sup>1</sup>; Inna Koukhareva<sup>1</sup>; Khaled Yamout<sup>1</sup>; <sup>1</sup>Trilink Biotechnologies, San Diego, CA
- WP 568 **Morpholino antisense oligonucleotides analyses using a compact matrix-assisted laser-desorption/ionization digital-ion-trap mass spectrometer (MALDI-DIT-MS);** Yuko Fukuyama<sup>1</sup>; Sadanori Sekiya<sup>1</sup>; Shinichi Iwamoto<sup>1</sup>; Koichi Tanaka<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan
- WP 569 **Investigating cyclic ion mobility as a means to boost coverage in the topdown sequencing of synthetic guide RNAs;** Catherine Tremblay<sup>1</sup>; Dale A Cooper-Shepherd<sup>2</sup>; Chris Knowles<sup>3</sup>; Michael Ruhl<sup>4</sup>; Christopher Gawlig<sup>4</sup>; James I. Langridge<sup>5</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>3</sup>Waters Corporation, Newcastle, United Kingdom; <sup>4</sup>Biospring GmbH, Frankfurt am Main, Germany; <sup>5</sup>Waters Corporation, Wilmslow, United Kingdom
- WP 570 **SEC x IP Two-Dimensional LCMS for the Analysis of Non-Denatured and Denatured Cyclic-Peptide siRNAs in a Single Step;** Stilianos G. Roussis<sup>1</sup>; Kristine Nguyen<sup>1</sup>; Claus Rentel<sup>1</sup>; <sup>1</sup>Ionis Pharmaceuticals, Inc., Carlsbad, CA
- WP 571 **Rapid Profiling of Impurities in Synthetic Oligonucleotides Using a Semi-Automated Data Analysis Workflow with ToF-MS;** Nick Pittman<sup>1</sup>; Ying Qing Yu<sup>2</sup>; Scott Berger<sup>2</sup>; Guillaume Bechade<sup>2</sup>; Kellen Delaney<sup>2</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Waters Corporation, Milford, MA
- WP 572 **Anion exchange chromatography fractionation of complex RNA mixtures for enhanced modification mapping via LC-MS/MS;** Cassandra Herbert<sup>1</sup>; Jennifer Kist<sup>1</sup>; Patrick A. Limbach<sup>1</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, OH
- WP 573 **Systematic Evaluation of Hydrophilic Interaction Liquid Chromatography Stationary Phases for Oligonucleotide Characterization by LC/MS;** Jordy J Hsiao<sup>1</sup>; Alex Apffel<sup>1</sup>; Lee Bertram<sup>1</sup>; Andrea Tripodi<sup>2</sup>; Andrew Coffey<sup>2</sup>; Ta-Chen Wei<sup>3</sup>; Connor Flannery<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Agilent Technologies Inc., Church Stretton, United Kingdom; <sup>3</sup>Agilent Technologies, Wilmington, DE
- WP 574 **Determination of Collision Cross-Sections of Nucleic Acids using an Orbitrap Mass Analyzer;** Jada N. Walker<sup>1</sup>; Jennifer S. Brodbelt<sup>1</sup>; <sup>1</sup>University of Texas at Austin, Austin, TX
- WP 575 **A Quantitative Competitive Transcription and Adduct Bypass Assay of Transcriptional Inhibition and Mutagenesis by O2-Alkylthymidine Lesions;** Chen



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- Wang<sup>1</sup>; Xiaomei He<sup>1</sup>; Yinan Wang<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- WP 576 **Global Analysis of Structured RNA-Protein Interactions using Stability-Based Mass Spectrometry Methods;** Morgan A. Bailey<sup>1</sup>; Justin G. Martyr<sup>2</sup>; Amanda E. Hargrove<sup>1,2</sup>; Michael C. Fitzgerald<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, Duke University, Durham, NC; <sup>2</sup>Department of Biochemistry, Duke University School of Medicine, Durham, NC
- WP 577 **Development of a SIM-based LCMS method for analysis of ribonucleoside mono-, di- and triphosphates and their mixtures;** Julio Hernandez Lopez<sup>1</sup>; Camila A Ortega<sup>1</sup>; Inna Koukhareva<sup>1</sup>; Khaled Yamout<sup>1</sup>; <sup>1</sup>Trilink Biotechnologies, San Diego, CA
- WP 578 **Impurity Profiling and Characterization of Therapeutic Oligonucleotides using Nominal Mass Spectrometry on a Single Quadrupole LC-UV-MS system;** Risa Suzuki<sup>1</sup>; Kosuke Uchiyama<sup>2</sup>; Noriko Kato<sup>2</sup>; Simon Ashton<sup>3</sup>; Neil J Loftus<sup>3</sup>; Yuka Fujito<sup>2</sup>; <sup>1</sup>SHIMADZU Corporation, Kawasaki, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Shimadzu Corporation, Manchester, United Kingdom
- WP 579 **Rapid monitoring of the purification process of oligonucleotide impurities using a benchtop MALDI-TOF MS system;** Takashi Nishikaze<sup>1</sup>; Kosuke Uchiyama<sup>1</sup>; Risa Suzuki<sup>2</sup>; Junji Kawakami<sup>3</sup>; Takao Inoue<sup>4</sup>; Satoshi Obika<sup>5</sup>; Yoshihiro Hayakawa<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>SHIMADZU Corporation, Kawasaki, Japan; <sup>3</sup>Konon University, Kobe, Japan; <sup>4</sup>National Institute of Health Sciences, Kawasaki, Japan; <sup>5</sup>Osaka university, Osaka, Japan
- WP 580 **Identification and functional characterizations of DNA N2-alkylguanine-binding proteins;** Ting Zhao<sup>1</sup>; Xiaomei He<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- WP 581 **Quantitative Analysis of a GalNAc-siRNA Conjugate and Its Metabolites Using Two-Dimensional Liquid Chromatography Coupled with Tandem Mass Spectrometry;** Li Fang<sup>1</sup>; Peiyun An<sup>1</sup>; Jinlian Lu<sup>1</sup>; Zhiyu Li<sup>1</sup>; Lili Xing<sup>1</sup>; Yi Tao<sup>1</sup>; Liang Shen<sup>1</sup>; <sup>1</sup>WuXi AppTec, Shanghai, China
- WP 582 **Characterization of 3'-poly(A)-tail length distribution in IVT-mRNA RNase A/T1 double digestions using sliding windows deconvolution;** Alexander Boris Schwahn<sup>1</sup>; Ken Cook<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, Reinach, Switzerland; <sup>2</sup>Thermo Fisher Scientific, Hemel Hempstead, United Kingdom
- WP 583 **High-throughput LC/MS characterization of mRNA therapeutics using a fast DDA method on the Orbitrap Astral MS;** Tabiwang Arrey<sup>1</sup>; Angela Criscuolo<sup>1</sup>; Keeley Murphy<sup>2</sup>; Eugen Damoc<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- WP 584 **Liquid Chromatography – Mass Spectrometry Characterization of siRNA Therapeutic Candidates: Workflows for siRNA Duplex Fidelity Assessment and Impurity Structure Elucidation;** Arseniy M Belov<sup>1</sup>; Yanjie Jiang<sup>1</sup>; Roy Huang<sup>1</sup>; Bo Pang<sup>1</sup>; Elena Belitsky<sup>1</sup>; <sup>1</sup>Alnylam Pharmaceuticals, Cambridge, MA
- WP 585 **Selective Characterization of mRNA 5' End Capping by LC-MS/MS using DNA Probe-Directed Enrichment with RNase 4;** Eric J. Wolf<sup>1</sup>; Nan Dai<sup>1</sup>; S. Hong Chan<sup>1</sup>; Ivan R. Corrêa Jr.<sup>1</sup>; <sup>1</sup>New England Biolabs, Inc., Beverly, MA
- WP 588 **Quantitation of a glucagon-like peptide-1 (GLP-1) analog in rat plasma using an LC-MS/MS workflow;** Amy Knight<sup>1</sup>; Ebru Selen<sup>1</sup>; Rahul Baghla<sup>1</sup>; Eshani Galermo<sup>1</sup>; <sup>1</sup>SCIEX, Redwood City, CA
- WP 589 **High-Throughput Characterization of Peptide Active Pharmaceutical Ingredient (API) Manufacturing Impurities by High-Resolution Ion Mobility Mass Spectrometry (HRIM-MS);** Ashli R Simone<sup>1</sup>; Sumukh Ray<sup>2</sup>; Michelle English<sup>1</sup>; Greg Kilby<sup>1</sup>; <sup>1</sup>MOBILion Systems, Chadds Ford, PA; <sup>2</sup>Bachem Americas, Inc., Vista, CA
- WP 590 **Quantitative Target Engagement for a KRAS G12C Inhibitor in FFPE Tumor Tissues using Immunoaffinity Capture 2D-LC-MRM;** Aiyng Yu<sup>1</sup>; Jintang He<sup>1</sup>; Lingyao Meng<sup>1</sup>; Zhen Shi<sup>1</sup>; Emily Chan<sup>1</sup>; Thomas Hunsaker<sup>1</sup>; Jian Jiang<sup>1</sup>; Surinder Kaur<sup>1</sup>; Keyang Xu<sup>1</sup>; <sup>1</sup>Genentech Inc, South San Francisco, CA
- WP 591 **Sensitive quantitation of glucagon-like peptide-1 (GLP-1) analog in rat plasma;** Tanya Gamble<sup>1</sup>; Ebru Selen<sup>2</sup>; Rahul Baghla<sup>2</sup>; Eshani Galermo<sup>2</sup>; <sup>1</sup>SCIEX, Concord, ON; <sup>2</sup>SCIEX, Redwood City, CA
- WP 592 **Quantitative Analysis of Protein Expression and Oxidative Damage in E. coli Strains Lacking Key Antioxidant Enzymes;** Yanjia Zhang<sup>1</sup>; Sanjay Kumar Rohaun<sup>2</sup>; James Imlay<sup>2</sup>; Aaron Timperman<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>University of Illinois at Urbana-Champaign, Urbana, IL
- WP 593 **Fit for purpose high-throughput absolute quantitation of chimeric aducanumab in mouse cortex and plasma;** Emma H Doud<sup>1</sup>; Katy Haynes<sup>2</sup>; Diogo Da Silva Dos Santos<sup>2</sup>; Jaison Arivalagan<sup>1</sup>; Amber L Mosley<sup>1</sup>; Sara Quinney<sup>1</sup>; Stacy J Sukoff Rizzo<sup>2</sup>; Paul Territo<sup>1,3</sup>; <sup>1</sup>Indiana University School of Medicine, Indianapolis, IN; <sup>2</sup>University of Pittsburgh, Pittsburgh, PA; <sup>3</sup>Indiana University Purdue University Indianapolis, Indianapolis, IN
- WP 594 **Applying targeted mass spectrometry to pulsed SILAC for protein turnover and quantitative proteomics;** Brooke Brauer<sup>1</sup>; AstraZeneca, Waltham, MA
- WP 595 **Capillary blood devices comparison for small peptide detection (<2 kDa) by LC-HRMS in antidoping analysis;** Carlotta Stacchini<sup>1</sup>; Fabio Comunità<sup>1</sup>; Xavier De La Torre<sup>1</sup>; Daniel Jardines<sup>1</sup>; Francesco Botrè<sup>1,2</sup>; <sup>1</sup>Antidoping Laboratory FMSI, Rome, Italy; <sup>2</sup>University of Lausanne, Lausanne, Switzerland
- WP 596 **Systematic quantification of rare misreading events in the bacterial inner membrane;** Nicola S. Freyer<sup>1</sup>; Nilanjan Ghosh Dastidar<sup>1</sup>; Ingo Wohlgemuth<sup>1</sup>; Henning Urlaub<sup>1,2</sup>; Marina V. Rodnina<sup>1</sup>; <sup>1</sup>Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; <sup>2</sup>University Medical Center Göttingen, Göttingen, Germany
- WP 597 **Evaluation of Parallel Reaction Monitoring Assays at Discovery Scale on a New Hybrid Nominal Mass Instrument for Phosphoproteomics Studies;** Cristina C. Jacob<sup>1</sup>; Hasmik Keshishian<sup>2</sup>; Alan Atkins<sup>3</sup>; Phillip M. Remes<sup>1</sup>; Michael W. Burgess<sup>2</sup>; Nikita Kormshchikov<sup>2</sup>; Claudia P.B. Martins<sup>1</sup>; Steven A. Carr<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Broad Institute, Cambridge, MA; <sup>3</sup>Thermo Fisher Scientific, Hemel Hempstead, United Kingdom
- WP 598 **Thermo Instrument Application Programming Interface enables on-the-fly adjustment of FAIMS compensation voltages for large-scale internal standard triggered PRM;** Nathan T Wamsley<sup>1</sup>; Michael B Major<sup>1</sup>; Dennis Goldfarb<sup>1</sup>; <sup>1</sup>Washington University in Saint Louis, St. Louis, MO
- WP 599 **The Targeted Tandem Mass Tag Experiment: A Tool for Accurate High Throughput Proteomics;** Philip M Remes<sup>1</sup>; Cristina C. Jacob<sup>1</sup>; Lilian R Heil<sup>1</sup>; Michael W. Senko<sup>1</sup>; Michael J. MacCoss<sup>2</sup>; Nicholas Shulman<sup>2</sup>; Brian Pratt<sup>2</sup>; Brendan MacLean<sup>2</sup>; Jae Choi<sup>3</sup>; Bhavin Patel<sup>3</sup>; Ryan Bomgarden<sup>3</sup>; Eric Zaniewski<sup>4</sup>; Johannes Kreuzer<sup>4</sup>; Lecia V Sequist<sup>4</sup>; Wilhelm Haas<sup>4</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>University of Washington - Genome Sciences, Seattle, WA; <sup>3</sup>Thermo Fisher Scientific, ROCKFORD, IL; <sup>4</sup>Massachusetts General Hospital (MGH), Charlestown, MA

**PEPTIDES: TARGETED AND QUANTITATIVE ANALYSIS**  
586-616

- WP 586 **Highly Sensitive and Multiplexed FAIMS-PRM Assays with Dynamic Retention Time and Organized FAIMS CVs for Clinical Applications;** Camille Lombard-Banek<sup>1</sup>; Yeoun Jin Kim<sup>2</sup>; Steve Sweet<sup>2</sup>; <sup>1</sup>Astrazeneca, Gaithersburg, MD; <sup>2</sup>AstraZeneca, Gaithersburg, MD
- WP 587 **Targeted peptide quantification with small foot-print capillary LC-MS/MS;** Xiaoli Dong<sup>1</sup>; Matthew Morse<sup>2</sup>; Greg Ward<sup>2</sup>; Linfeng Wu<sup>1</sup>; Patrick Batoon<sup>1</sup>; Maozi Liu<sup>3</sup>; <sup>1</sup>Agilent, Santa Clara, CA; <sup>2</sup>Axced, Provo, UT; <sup>3</sup>Agilent Technologies, Santa Clara, CA

## WEDNESDAY POSTERS

- WP 600 **Targeted measurements enable robust quantitation of low-abundance proteins from single cells;** H. Lavender Lin<sup>1</sup>; Lilian R Heil<sup>2</sup>; Fernanda Salvato<sup>2</sup>; Philip M. Remes<sup>2</sup>; Cristina C. Jacob<sup>2</sup>; Amirmansoor Hakim<sup>2</sup>; Tonya Pekar Hart<sup>2</sup>; Ryan T. Kelly<sup>1</sup>; <sup>1</sup>Brigham Young University, Provo, UT; <sup>2</sup>ThermoFisher Scientific, San Jose, CA
- WP 601 **Interrogating the heart disease-relevant protein isoform landscape of smooth muscle cells using mass spectrometry;** Jennifer A Korchak<sup>1</sup>; Erin Jeffery<sup>1</sup>; Mayank Murali<sup>1,2</sup>; Noah Perry<sup>1</sup>; Mete Civelek<sup>1</sup>; Gloria Sheynkman<sup>1</sup>; <sup>1</sup>University of Virginia, Charlottesville, VA; <sup>2</sup>Broad Institute of MIT and Harvard, Cambridge, MA
- WP 602 **High Throughput Peptide Purification Strategies using Silica-based 96-Well SPE Formats Prior LC-MS Analysis;** Elizabeth Denton<sup>1</sup>; Amit Mehrotra<sup>1</sup>; <sup>1</sup>Biotage, Charlotte, NC
- WP 603 **LC-MRM-based assay for quantitative assessment of fibrinogen levels in clinical samples;** Sandip Chavan<sup>1</sup>; Ramesh Bokka<sup>1</sup>; Shilpa Venkataraman<sup>1</sup>; Jane Peterson<sup>1</sup>; Julie Tange<sup>1</sup>; Rachel Leger<sup>1</sup>; Jansen Seheult<sup>1</sup>; Rajiv Pruthi<sup>1</sup>; Dong Chen<sup>1</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN
- WP 604 **Quantitative LC-MS/MS Analysis of Exogenously Administered Oxytocin in Pediatric Patients;** Jeff Jeppson<sup>1</sup>; Lee Winchester<sup>1</sup>; Anthony Podany<sup>1</sup>; Christopher Shaffer<sup>1</sup>; <sup>1</sup>UNMC, Omaha, NE
- WP 605 **Mapping start codons of small open reading frames by N-terminomics approach;** Cuihong Wan; <sup>1</sup>Central China Normal University, Wuhan, China
- WP 606 **Inheritance in wet-dry cycling based Prebiotic Evolving Chemical Systems;** Kavita R Matange<sup>1</sup>; Vahab Rajaei<sup>1</sup>; Loren Dean Williams<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA
- WP 607 **Utilizing the power of the timsTOF Ultra for targeted PRM analysis;** Casey Powers<sup>1</sup>; Allis Chien<sup>2</sup>; Ryan Leib<sup>2</sup>; Fang Liu<sup>2</sup>; <sup>1</sup>Stanford University, Stanford, CA; <sup>2</sup>Stanford University Mass Spectrometry, Stanford, California
- WP 608 **High-Throughput Subclass-Specific Glycan Profiling of Human Serum IgG Using Parallel Reaction Monitoring Peptide Bond Fragmentation of Glycopeptides and Microflow LC-MS;** Shivkumar Raidas<sup>1</sup>; Yunlong Zhao<sup>1</sup>; Yuan Mao<sup>1</sup>; Ning Li<sup>1</sup>; <sup>1</sup>Regeneron Pharmaceuticals, Inc., Tarrytown, NY
- WP 609 **Charged-Surface Stationary Phase Improves Peptide Peak Shape in Low Ionic Strength Mobile Phases;** Benjamin Libert<sup>1</sup>; Barry Boyes<sup>1</sup>; Chuping Luo<sup>1</sup>; <sup>1</sup>Advanced Materials Technology, Wilmington, DE
- WP 610 **Sub-Picogram Level Bio-Analytical Method for Quantification of Desmopressin in Human Plasma Using LCMS-8060NX;** Chaitanya Krishna Atmakuri<sup>1</sup>; Avinash B Gaikwad<sup>1</sup>; Yogesh G Arote<sup>1</sup>; <sup>1</sup>ADC-Shimadzu Analytical India Pvt Ltd, NAVI MUMBAI, India
- WP 611 **Scout triggered MRM : a method to acquire large numbers of MRM without predefined retention time;** Holly Lee<sup>1</sup>; David Cox<sup>1</sup>; Yves Le Blanc<sup>2</sup>; <sup>1</sup>SCIEX, Concord, ON; <sup>2</sup>SCIEX, Concord, On, ON
- WP 612 **Precise and accurate quantitation of critical host cell proteins (HCPs) using a targeted peptide mixture and LC-MS/MS analysis;** Noelia De Lama<sup>1,2</sup>; Corentin Beaumal<sup>1,2</sup>; Jae Choi<sup>3</sup>; Bhavin Patel<sup>3</sup>; Nikki Jarrett<sup>3</sup>; Kay Opperman<sup>3</sup>; Christine Carapito<sup>1,2</sup>; <sup>1</sup>Laboratoire de Spectrométrie de Masse BioOrganique, IPHC (UMR 7178), CNRS, Strasbourg, France; <sup>2</sup>Infrastructure Nationale de Protéomique ProFI – FR2048, Strasbourg, France; <sup>3</sup>Thermo Fisher Scientific, ROCKFORD, IL
- WP 613 **A Rapid Liquid Chromatography-Mass Spectrometry Quantitation of Somatostatin in Rat Plasma;** Yongqing He<sup>1</sup>; Zhenhua Jiang<sup>1</sup>; Lizhi Guo<sup>1</sup>; Nan Zhao<sup>1</sup>; Zhiyu Li<sup>1</sup>; Lili Xing<sup>1</sup>; Yi Tao<sup>1</sup>; Liang Shen<sup>1</sup>; <sup>1</sup>WuXi AppTec, Shanghai, China
- WP 614 **Comprehensive quantitation of the mitochondrial proteome with parallel reaction monitoring and real-time retention alignment;** Valerie N. Lynch<sup>1</sup>; Lilian R Heil<sup>2</sup>; Chris McGann<sup>1</sup>; Erik Bergstrom<sup>1</sup>; Philip M Remes<sup>2</sup>; Cristina C. Jacob<sup>2</sup>; Devin K Schweppe<sup>1</sup>; <sup>1</sup>University of Washington - Genome Sciences, Seattle, WA; <sup>2</sup>ThermoFisher Scientific, San Jose, CA
- WP 615 **The power of the multi-attribute method in advancing novel modalities in process and product development;** Vamsikrishna Kandhi<sup>1</sup>; Keith Johnson<sup>1</sup>; <sup>1</sup>Pfizer Inc., Andover, MA
- WP 616 **Optimizing DIA and PRM workflows for the Orbitrap Astral mass spectrometer;** Marcel Morgenstern<sup>1,2</sup>; Benton J Anderson<sup>1,2</sup>; Noah Michael Lancaster<sup>1,3</sup>; Corinne Moss<sup>1</sup>; Margaret Lea Robinson<sup>1</sup>; Pavel Sinitcyn<sup>4</sup>; Joshua J Coon<sup>1,2,3,4</sup>; <sup>1</sup>Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI; <sup>3</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>4</sup>Morgridge Institute for Research, Madison, WI

### PROTEIN THERAPEUTICS: QUANTITATIVE ANALYSIS 617-641

- WP 617 **Double Immunocapture-LC/MS/MS Assay Method Development and Validation in Support of BI-X GLP Monkey Ocular Studies;** Bailuo Ren<sup>1</sup>; Yan Mao<sup>1</sup>; David Roos<sup>1</sup>; Kelly Coble<sup>1</sup>; <sup>1</sup>Boehringer Ingelheim, Ridgefield, CT
- WP 618 **Nontraditional IC-LC/MS Method Development and Bioanalysis for On Demand Cytokines;** Emily Werth<sup>1</sup>; Elsy Philip<sup>1</sup>; Tammy Bigwarfe<sup>1</sup>; Kelly Coble<sup>1</sup>; <sup>1</sup>Boehringer Ingelheim, Ridgefield, CT
- WP 619 **A Spectra library assisted workflow for host cell protein detection and quantitation in recombinant peptide drug products by CapLC-HRMS/MS;** Cung N Thawng<sup>1</sup>; Cynthia Sommers<sup>1</sup>; Eric Pang<sup>2</sup>; David A Keire<sup>1</sup>; Hongbin Zhu<sup>3</sup>; <sup>1</sup>U.S. FDA, St Louis, MO; <sup>2</sup>U.S. Food and Drug Administration, Silver Spring, MD; <sup>3</sup>U.S. FDA, Saint Louis, MO
- WP 620 **An Approach for Multi Attribute Monitoring of Bi-Specific Antibodies Employing Capillary Electrophoresis and Intact Mass Spectrometry;** Nancy Fernandes; Lonza, Portsmouth, NH
- WP 621 **Implementing Microflow LC-MS/MS for Quantification of Antibody-drug Conjugates and Biotherapeutic Proteins During Early Drug Discovery and Development;** Joshua B Powers<sup>1</sup>; Moo-jin Suh<sup>1</sup>; <sup>1</sup>AstraZeneca, Gaithersburg, MD
- WP 622 **Investigate the Antileukemic Effect of the Synthetic Retinoid ST1926 in HTLV-1 Positive and Negative Malignant T Cells using LC-MS/MS Proteomics;** Mona Goli<sup>1</sup>; Mojibola Fowowe<sup>1</sup>; Vishal Sandilya<sup>1</sup>; Botheina Ghandour<sup>2</sup>; Firas Kobeissy<sup>2,3</sup>; Nadine Darwiche<sup>2</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Chemistry and Biochemistry Department, Texas Tech University, Lubbock, TX; <sup>2</sup>Department of Biochemistry and Molecular Genetics, American University of Beirut, Beirut, Lebanon; <sup>3</sup>Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA
- WP 623 **Antibody guanidination: an alternative antibody internal standard approach to antibody quantification in canine plasma using IA LC-MS/MS;** Drupadkumar Acharya<sup>1</sup>; Henry Li<sup>1</sup>; Wei Tong<sup>1</sup>; Laura Letendre<sup>1</sup>; <sup>1</sup>Boehringer Ingelheim Animal Health USA Inc., North Brunswick, NJ
- WP 624 **Develop and Validate a Universal LC-MS/MS Assay to Quantify Succinylated Genes in Human Plasma to Support BE Studies;** Yuhuan Ji<sup>1</sup>; Changgang Li<sup>1</sup>; Changjian Zhao<sup>1</sup>; Min Meng<sup>1</sup>; Laixin Wang<sup>1</sup>; <sup>1</sup>Resolian China, Chongqing, China
- WP 625 **Multi-Omics Investigation of Biotherapeutic Expressing CHO Cell Lines In Fed Batch Bioreactors;** Charles Eldrid<sup>1</sup>; Ellie Hawke<sup>1</sup>; Lee A Gethings<sup>2</sup>; John Raven<sup>3</sup>; Richard Lock<sup>2</sup>; Joanna Watson<sup>1</sup>; Alan Dickson<sup>1</sup>; James I. Langridge<sup>2</sup>; Leon Pybus<sup>3</sup>; Andrew Pitt<sup>1</sup>; Perdita Barran<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, United Kingdom; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>3</sup>FUJIFILM Diosynth Biotechnologies UK, Billingham, United Kingdom
- WP 626 **Coupling Enrichment and Depletion Methods with FAIMS-MS for Enhanced Host Cell Protein Identification in Biotherapeutic Development;** Christopher Sauer<sup>1</sup>; Abby J. Chiang<sup>2</sup>; Elsa Gorre<sup>1</sup>; Andrew D Mahan<sup>1</sup>; Hirsh Nanda<sup>1</sup>;

## WEDNESDAY POSTERS

- <sup>1</sup>Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania; <sup>2</sup>Protein Metrics, LLC, Cupertino, CA
- WP 627 **Design of Experiment Assisted Method Development and Validation of Quantitative Immunoaffinity-capture LC-MS/MS Assay for Therapeutic Proteins in Human Serum;** Yan-Ping Lin<sup>1</sup>; Anisha Rai<sup>1</sup>; Shuyu Hou<sup>1</sup>; Tian-Sheng Lu<sup>1</sup>; <sup>1</sup>Medpace, Cincinnati, OH
- WP 628 **Automated 96-well desalting and collision induced unfolding analysis of biotherapeutics;** Michael R Armbruster<sup>1</sup>; Amanda Cicali<sup>1</sup>; Tyler Somerville<sup>1</sup>; Nicole A Rivera-Fuentes<sup>1</sup>; Youngseo Na<sup>2</sup>; Alyssa Erlenbeck<sup>1</sup>; Anna Schwendeman<sup>3</sup>; Brandon T Ruotolo<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Michigan, Ann Arbor, Michigan; <sup>2</sup>Department of Medicinal Chemistry, University of Michigan, Ann Arbor, MI; <sup>3</sup>Department of Pharmaceutical Sciences, University of Michigan, Ann Arbor, MI
- WP 629 **Development of a novel middle-up HILIC-MS method for intra-domain free thiol localization and quantitation in therapeutic monoclonal antibodies;** Xin Wang<sup>1</sup>; Xiaoxiao Huang<sup>1</sup>; Shunhai Wang<sup>1</sup>; Ning Li<sup>1</sup>; <sup>1</sup>Regeneron Pharmaceuticals, Inc., Tarrytown, NY
- WP 630 **Intact Mass Analysis for the Quantitation of Free Subunits Observed in Antibody-based Proteins;** Kyoung-Soo Choi<sup>1</sup>; Pooja Madhav Raju<sup>1</sup>; Helen Zou<sup>1</sup>; John Patrick<sup>1</sup>; Steven Pomerantz<sup>1</sup>; Tun Liu<sup>1</sup>; Richard Huang<sup>1</sup>; <sup>1</sup>Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania
- WP 631 **A Single, Integrated Software Platform for LC/MS-based Multi-Attribute Method (MAM) Approaches, with Automated Review;** Aude Tartiere<sup>1</sup>; Can Cui<sup>2</sup>; Catherine Evans<sup>3</sup>; Stephen Kok<sup>1</sup>; Yaarub Musa<sup>3</sup>; Arnd Brandenburg<sup>3</sup>; <sup>1</sup>Genedata Inc, San Francisco, CA; <sup>2</sup>Genedata Inc., Lexington, Massachusetts; <sup>3</sup>Genedata AG, Basel, Switzerland
- WP 632 **Regulated Bioanalysis for Large Peptide/Small Protein Quantitation in Matrix by LC-MS: Can We Detect Intact or Digested Peptide?;** Moucun Yuan<sup>1</sup>; Kumar Shah<sup>1</sup>; Gang Xu<sup>1</sup>; Gus Hui<sup>1</sup>; M. Shane Woolf<sup>1</sup>; William R. Mylott Jr. 1; <sup>1</sup>PPD, part of Thermo Fisher Scientific, Richmond, VA
- WP 633 **Identification and Quantitation of Heterodimers in Co-Formulated Monoclonal Antibody Cocktails: From Sample Treatment Strategies to Native SEC-MS Analysis;** Wenjing Peng<sup>1</sup>; Yuetian Yan<sup>1</sup>; Victoria C. Cotham<sup>1</sup>; Shunhai Wang<sup>1</sup>; Ning Li<sup>1</sup>; <sup>1</sup>Regeneron Pharmaceuticals, Inc., Tarrytown, NY
- WP 634 **Development of an LC-MS/MS Assay for Quantitative Analysis of the Biotherapeutic Protein that Overcomes the ADA Impact in Human Serum;** Gang Xu<sup>1</sup>; Joe Palandra<sup>2</sup>; Kumar Shah<sup>1</sup>; Moucun Yuan<sup>1</sup>; Gus Hui<sup>1</sup>; William R. Mylott Jr. 1; M. Shane Woolf<sup>1</sup>; Mike Baratta<sup>2</sup>; <sup>1</sup>PPD, part of Thermo Fisher Scientific, Richmond, VA; <sup>2</sup>Takeda Development Corporation, Americas, Cambridge, MA
- WP 635 **Localization of PTMs on Multi Specific antibody through Middle down analysis by Microfluidic Chip-Based Integrated icIEF-UV/MS technology;** Kristen Niels<sup>1</sup>; Hirsh Nanda<sup>2</sup>; Scott Mack<sup>3</sup>; Zoe Zhang<sup>4</sup>; Mariam S ElNaggar<sup>3</sup>; Megan E. Sharma<sup>2</sup>; Riley Schaeffer<sup>2</sup>; Robert Hepler<sup>2</sup>; <sup>1</sup>Janssen Biopharmaceuticals, Springhouse, PA; <sup>2</sup>Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania; <sup>3</sup>SCIEX, Fremont, CA; <sup>4</sup>SCIEX, Redwood City, CA
- WP 636 **De Novo Sequencing and Assembly of Multiclonal Nanobodies;** Qingyang Xiao<sup>1</sup>; Sujun Li<sup>1</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN
- WP 637 **Exploiting Isotope Resolution of Intact Protein Mass Spectra with Gábor Transform for Improved Multi-Protein Deconvolution and Accurate, Automated Antibody Quantitation;** Kayd L. Meldrum<sup>1</sup>; Andrew K. Swansiger<sup>1</sup>; Meghan Daniels<sup>1</sup>; Crystal Kirmiz Cody<sup>2</sup>; David L. Wong<sup>2</sup>; Mike Knierman<sup>2</sup>; Xi Qiu<sup>2</sup>; John Sausen<sup>2</sup>; Anthony D. Maus<sup>3</sup>; Paula M. Ladwig<sup>3</sup>; Maria A. V. Willrich<sup>3</sup>; James S. Prell<sup>1, 4</sup>; <sup>1</sup>University of Oregon, Eugene, OR; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>Mayo Clinic, Rochester, MN; <sup>4</sup>Materials Science Institute, University of Oregon, Eugene, OR
- WP 638 **Nano LC/MS based quantitative assessment of the processing of a novel conditionally active bispecific T-cell engager in monkey plasma;** Yipei Zhang<sup>1</sup>; Mark G. Qian<sup>1</sup>; Linlin Dong<sup>1</sup>; <sup>1</sup>Takeda Development Corporation, Americas, Cambridge, MA
- WP 639 **Interlaboratory study for characterizing NISTmAb by microfluidic chip-based integrated imaged capillary isoelectric focusing (icIEF)-UV/MS;** Mariam S ElNaggar<sup>1</sup>; Kristen Niels<sup>2</sup>; Kristine F Parson<sup>3</sup>; Anita P Liu<sup>4</sup>; Xiaoping Z He<sup>5</sup>; Tony Cozzolino<sup>6</sup>; James Ingersoll<sup>7</sup>; Steven Chow<sup>1</sup>; Rita Nichiporuk<sup>1</sup>; Jose-Luis Gallegos-Perez<sup>6</sup>; Zhenjiu Liu<sup>5</sup>; Zac VanAernum<sup>4</sup>; Margo Wilson<sup>3</sup>; Riley Schaeffer<sup>2</sup>; Seung-Yong Jung<sup>1</sup>; Jackie Le<sup>1</sup>; Rashmi Madda<sup>7</sup>; Megan E. Sharma<sup>2</sup>; Daniel Zorzon<sup>7</sup>; Fred Mannarino<sup>7</sup>; Sisi Huang<sup>5</sup>; Michael Merriman<sup>7</sup>; Alexander Petrov<sup>1</sup>; Scott Mack<sup>1</sup>; Daniel French<sup>7</sup>; John Orlet<sup>8</sup>; Jingwen Ding<sup>1</sup>; Alcenir Soares<sup>7</sup>; Chelsea Leonce<sup>2</sup>; Jennifer Chui<sup>1</sup>; Matthew Heindel<sup>7</sup>; Tom Lerch<sup>8</sup>; Haichuan Liu<sup>7</sup>; Thomas Powers<sup>9</sup>; Wei Chen<sup>1</sup>; Lien Kwan<sup>7</sup>; Vincent Vang<sup>1</sup>; Johan Hermansson<sup>7</sup>; Melissa Anderson<sup>8</sup>; Tristan Williams<sup>7</sup>; <sup>1</sup>SCIEX, Fremont, CA; <sup>2</sup>Janssen Research and Development, Spring House, PA; <sup>3</sup>FUJIFILM Diosynth Biotechnologies USA, Inc, Morrisville, NC; <sup>4</sup>Merck, Kenilworth, NJ; <sup>5</sup>Pfizer, Chesterfield, MO; <sup>6</sup>Sciex, Framingham, MA; <sup>7</sup>SCIEX, Redwood City, CA; <sup>8</sup>Pfizer Inc., Chesterfield, MO; <sup>9</sup>Pfizer Inc, Chesterfield, MO
- WP 640 **Quantifying epitope-specific affinities of naturally acquired antibodies to a malaria protein using native mass spectrometry;** Daniel Ferrer Vinals<sup>1</sup>; Duong T. Bui<sup>2</sup>; Mohammad R. Hoque<sup>1</sup>; Eliana Arango<sup>3</sup>; Amanda Maestre<sup>3</sup>; Lara K. Mahal<sup>2</sup>; Stephanie K. Yanow<sup>1</sup>; John S. Klassen<sup>2</sup>; <sup>1</sup>School of Public Health, University of Alberta, Edmonton, AB; <sup>2</sup>Department of Chemistry, University of Alberta, Edmonton, AB; <sup>3</sup>Grupo Salud y Comunidad, Facultad de Medicina, Universidad de Antioquia, Medellin, Colombia
- WP 641 **New tools for biologics analyses and QC: the Shredder and S-Trap Turbo MAM;** Stefan Loroch<sup>1,2</sup>; Sandra Wilson<sup>1</sup>; Alexandre Zougman<sup>3</sup>; John P Wilson<sup>1</sup>; <sup>1</sup>Protifi, LLC, Fairport, NY; <sup>2</sup>Ruhr-University Bochum, Bochum, Germany; <sup>3</sup>University of Leeds, Leeds, United Kingdom

### PROTEINS: GENERAL AND MEMBRANE 642-657

- WP 642 **Mass Spectrometric Identification of Invasion Receptors on Red Blood Cell Precursors for the Malaria Parasite Plasmodium vivax;** Jessica S Molina<sup>1</sup>; Daniel Roeth<sup>1</sup>; Manuel Alfonso Pataroyo<sup>2</sup>; Markus Kalkum<sup>1</sup>; <sup>1</sup>City of Hope, Duarte, CA; <sup>2</sup>Fundación Instituto de Inmunología de Colombia, Bogotá, Colombia
- WP 643 **Enhanced Signal Processing Methods for Membrane Protein Collision Induced Unfolding Analysis;** Iliana Levesque<sup>1</sup>; Kristine F. Parson<sup>2</sup>; Sarah M. Fantin<sup>3</sup>; Aniruddha Panda<sup>4</sup>; Kallol Gupta<sup>4</sup>; Brandon T. Ruotolo<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, Michigan; <sup>2</sup>FUJIFILM Diosynth Biotechnologies USA, Inc, Morrisville, North Carolina; <sup>3</sup>Hanover College, Hanover, Indiana; <sup>4</sup>Yale University, West Haven, CT
- WP 644 **Development of Mass Spectrometry Grade Membrane Protein Standard;** Alyson Jesionowski<sup>1</sup>; Leigh Foster<sup>1</sup>; Aaron McBride<sup>1</sup>; Joanna Geddes<sup>1</sup>; Kay Opperman<sup>1</sup>; Barbara Kaboord<sup>1</sup>; Bhavin Patel<sup>1</sup>; Weijing Liu<sup>2</sup>; Yuqi Shi<sup>2</sup>; Rosa Viner<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, Rockford, IL; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- WP 645 **Studies of Aquaporin-0 Lipid Binding in the Bovine Lens via Native Mass Spectrometry;** Carla V.T. O'Neale<sup>1</sup>; Sophie R. Harvey<sup>2</sup>; Vicki H. Wysocki<sup>2</sup>; Kevin L. Schey<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>The Ohio State University, Columbus, OH
- WP 646 **Analysis of Membrane Proteins under Native and Denaturing Conditions Using Capillary Electrophoresis Coupled to High-Resolution Mass Spectrometry;** Noah Gould<sup>1</sup>; Yunfan Gao<sup>1</sup>; Michal Gregus<sup>1</sup>; Kendall R Johnson<sup>1</sup>;

## WEDNESDAY POSTERS

- Anne-Lise Marie<sup>1</sup>; Alexander R. Ivanov<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*
- WP 647 **A comparison of sample preparation, data acquisition and data processing workflows for untargeted bottom-up plasma proteomics**; Carina Lima<sup>1</sup>; Leanne Ohlund<sup>1</sup>; Kevin Ly<sup>2</sup>; Maxim Isabelle<sup>2</sup>; Victoria Miller<sup>2</sup>; Hugo Gagnon<sup>2</sup>; Lekha Sleno<sup>1</sup>; <sup>1</sup>*UQAM, Montreal, QC*; <sup>2</sup>*Allumiqs, Sherbrooke, QC*
- WP 648 **Unbiased characterization of GPCRs spatiotemporal activities revealed novel receptor trafficking and signaling signatures**; Qiongyu Li<sup>1</sup>; Benjamin Polacco<sup>1</sup>; Martin Gordon<sup>1</sup>; Trupti Patil<sup>1</sup>; Aaron Marley<sup>1</sup>; Prachi Khare<sup>1</sup>; Jiewei Xu<sup>1</sup>; Xiaofang Zhong<sup>1</sup>; Emily Blythe<sup>1</sup>; Aliza Ehrlich<sup>1</sup>; Kirsten Obenier<sup>1</sup>; Nevan Krogan<sup>1</sup>; Mark Von Zastrow<sup>1</sup>; Ruth Huttenhain<sup>1,2</sup>; <sup>1</sup>*University of California, San Francisco, San Francisco, CA*; <sup>2</sup>*Stanford University, Palo Alto, CA*
- WP 649 **Characterization of Insect Sperm Nuclear Basic Proteins by Liquid Chromatography – Tandem Mass Spectrometry**; Melissa R Leyden<sup>1</sup>; Donald F. Hunt<sup>1</sup>; Jeffrey Shabanowitz<sup>1</sup>; <sup>1</sup>*University of Virginia, Charlottesville, VA*
- WP 650 **Unveiling the SEA Domain Self-Cleavage of GPR110 and its Impact on GAIN Domain Autoproteolysis: Insights from Quantitative Mass Spectrometry**; Bill Huang<sup>1</sup>; Hee-Yong Kim<sup>1</sup>; <sup>1</sup>*NIAAA/NIH, Rockville, MD*
- WP 651 **A lipid vesicle ion mobility-mass spectrometry platform uncovers how membrane protein-lipid organization at the synaptic membrane drives ultrafast neurotransmitter release**; Aniruddha Panda<sup>1</sup>; Iliana Levesque<sup>2</sup>; Anna L. Duncan<sup>3</sup>; Jean N.D. Goder<sup>1</sup>; Frederic Pincet<sup>4</sup>; Brandon T Ruotolo<sup>5</sup>; Kallol Gupta<sup>1</sup>; <sup>1</sup>*Department of Cell Biology, Yale University, West Haven, CT*; <sup>2</sup>*Department of Chemistry, University of Michigan, Ann Arbor, MI*; <sup>3</sup>*Department of Chemistry, Aarhus University, Aarhus, Denmark*; <sup>4</sup>*Laboratoire de Physique de l'Ecole Normale Supérieure, ENS, CNRS, Université PSL, Sorbonne Université, Université Paris-Cité, Paris, France*; <sup>5</sup>*Department of Chemistry, University of Michigan, Ann Arbor, Michigan*
- WP 652 **Analysis of Whole Cell Yeast Lysates by Charge Detection Mass Spectrometry**; Nick Rommel<sup>1</sup>; Adam Anthony<sup>1</sup>; David Clemmer<sup>1</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*
- WP 653 **Characterizing Ligand Binding to the AmtB/GlnK Complex using Direct Mass Technology**; Jared Hampton<sup>1</sup>; Robert L. Schrader<sup>1</sup>; Robert Rider<sup>1</sup>; Smriti Kumar<sup>1</sup>; Carter Lantz<sup>1</sup>; David H Russell<sup>1</sup>; <sup>1</sup>*Texas A&M University, College Station, TX*
- WP 654 **A high-throughput proteome-wide platform for capturing membrane proteins in their native environment for structural and functional studies**; Caroline Brown<sup>1</sup>; Snehasish Ghosh<sup>1</sup>; Yansheng Liu<sup>2</sup>; Moitrayee Bhattacharyya<sup>2</sup>; Kallol Gupta<sup>1</sup>; <sup>1</sup>*Yale School of Medicine, Department of Cell Biology, New Haven, CT*; <sup>2</sup>*Yale School of Medicine, Department of Pharmacology, New Haven, CT*
- WP 655 **Whole proteome analysis of endothelial cells in response to catecholamine stimulation using an untargeted approach**; Amar Ingi Vilhjalmsson<sup>1</sup>; Óttar Rolfsson<sup>1</sup>; <sup>1</sup>*University of Iceland, Reykjavik, Iceland*
- WP 656 **nanoCSC reveals novel insight into the surfaceome of primary human cardiomyocytes in heart failure**; Roneldine Mesidor<sup>1</sup>; Melinda Wojtkiewicz<sup>1</sup>; Michelle Waknitz<sup>1</sup>; Rebekah L Gundry<sup>1</sup>; <sup>1</sup>*University of Nebraska Medical Center, Omaha, NE*
- WP 657 **HiBIT Protein Tagging System for Quantitative Study of Protein Dynamics at Endogenous Levels**; Virginia Kincaid<sup>1</sup>; Christopher Eggers<sup>1</sup>; Mike Rosenblatt<sup>1</sup>; Brock Binkowski<sup>1</sup>; Marjeta Urh<sup>1</sup>; <sup>1</sup>*Promega Corporation, Madison, WI*
- Worth<sup>1</sup>; Joseph H Taube<sup>1</sup>; Elyssia S Gallagher<sup>1</sup>; <sup>1</sup>*Baylor University, Waco, TX*
- WP 659 **PTMeXchange species specific PTM builds: Meta-analysis of datasets and dissemination of high-quality PTM data for community use**; Kerry A Ramsbottom<sup>1</sup>; Ellen Boswell<sup>1</sup>; Oscar M Camacho<sup>1</sup>; Shireen Al-Momani<sup>1</sup>; Ananth Prakash<sup>2</sup>; Yasset P Riverol<sup>2</sup>; Zhi Sun<sup>3</sup>; Deepti J Kundu<sup>2</sup>; Emily Bowler-Barnett<sup>2</sup>; Maria Martin<sup>2</sup>; Jun Fan<sup>2</sup>; Eric W Deutsch<sup>3</sup>; Juan Antonio Vizcaino<sup>2</sup>; Andrew R. Jones<sup>1</sup>; <sup>1</sup>*University of Liverpool, Liverpool, United Kingdom*; <sup>2</sup>*European Bioinformatics Institute, Cambridge, United Kingdom*; <sup>3</sup>*Institute for Systems Biology, Seattle, Washington*
- WP 660 **Deciphering the Notch signalling pathway using magnetic beads coupled with delta ligands and quantitative phosphoproteomics**; Michael Savnisch<sup>1,2</sup>; Levent Marcel Oelmez<sup>1,2</sup>; Marcus Krüger<sup>1,2</sup>; Luisa Schmidt<sup>1,2</sup>; Jan-Wilim Lackmann<sup>1,2</sup>; Stefan Müller<sup>1,2</sup>; <sup>1</sup>*University of Cologne, Cologne, Germany*; <sup>2</sup>*CECAD (Cluster of Excellence in Cellular Stress Responses in Aging-Associated Diseases), Cologne, Germany*
- WP 661 **Assessment of aging profile of archaeological animal bone collagen in terms of glutamine deamidation using mass spectrometry**; Takashi Nakazawa<sup>1</sup>; Masaru Miyagi<sup>2</sup>; Kazuki Kawahara<sup>3</sup>; Seiji Kadowaki<sup>4</sup>; Yoshihiro Nishiaki<sup>5</sup>; <sup>1</sup>*Nara Women's University, Nara, Japan*; <sup>2</sup>*Case Western Reserve University, Cleveland, Ohio*; <sup>3</sup>*Osaka University, Suita, Japan*; <sup>4</sup>*Nagoya University, Nagoya, Japan*; <sup>5</sup>*The University of Tokyo, Bunkyo-ku, Japan*
- WP 662 **Ethanol-induced post-translational acetylation alters hepatic metabolism in mice**; Mirjavid Aghavey<sup>1</sup>; Sergeui Ilchenko<sup>1</sup>; Victor Lufi<sup>1</sup>; Jack Mathis<sup>1</sup>; Megan McMullen<sup>2</sup>; Hannah Marchuk<sup>3</sup>; Tsung-Heng Tsai<sup>4</sup>; Guofang Zhang<sup>3</sup>; Laura Nagy<sup>2</sup>; Takhar Kasumov<sup>1</sup>; <sup>1</sup>*Northeast Ohio Medical University, Rootstown, OH*; <sup>2</sup>*Cleveland Clinic, Cleveland, OH*; <sup>3</sup>*Duke University, Durham, NC*; <sup>4</sup>*Kent State University, Kent, OH, 44240*
- WP 663 **Automated and Robust Identification of Scrambled Disulfide Bonds in Biotherapeutics**; Stephen Kok<sup>1</sup>; Aude Tartiere<sup>1</sup>; Can Cui<sup>2</sup>; Catherine Evans<sup>3</sup>; Yaarub Musa<sup>3</sup>; Arnd Brandenburg<sup>3</sup>; <sup>1</sup>*Genedata Inc, San Francisco, CA*; <sup>2</sup>*Genedata Inc., Boston, MA*; <sup>3</sup>*Genedata AG, Basel, Switzerland*
- WP 664 **Mapping functions of diphthamide biosynthetic enzymes using multiple proteomic approaches**; Lauren Mazurkiewicz<sup>1</sup>; Amy Weeks<sup>1</sup>; <sup>1</sup>*University of Wisconsin-Madison, Madison, WI*
- WP 665 **HiNT erases AMPylation and GMPylation from proteins revealed by mass spectrometric analysis**; Yanping Qiu<sup>1</sup>; Heenam Park<sup>1</sup>; Chieh-Hsiang Tan<sup>1</sup>; Baiyi Quan<sup>1</sup>; Paul W. Sternberg<sup>1</sup>; Tsui-Fen Chou<sup>1</sup>; <sup>1</sup>*Caltech, Pasadena, CA*
- WP 666 **Definitive Identification of Sulfation in an Antibody SEFL1 Motif by High Resolution Mass Spectrometry with Site Identification by ETHcD MS/MS**; John H. Robinson<sup>1</sup>; Shuai Wu<sup>1</sup>; Iain D.G. Campuzano<sup>1</sup>; <sup>1</sup>*Amgen Inc., Thousand Oaks, CA*
- WP 667 **Formation of Cys-TMT from Interaction of iodoTMT0 with Cysteine Residues Alkylated by N-Ethylmaleimide (NEM)**; Jian Cai<sup>1</sup>; Ming Song<sup>2,3</sup>; Ming Li<sup>1</sup>; Michael Merchant<sup>1</sup>; Frederick Benz<sup>4</sup>; Craig McClain<sup>2,3,4,5,6</sup>; Jon Klein<sup>1,5,11</sup>; <sup>1</sup>*Division of Nephrology and Hypertension, Department of Medicine, University of Louisville School of Medicine, Louisville, Kentucky*; <sup>2</sup>*Division of Gastroenterology, Hepatology and Nutrition, Department of Medicine, University of Louisville School of Medicine, LOUISVILLE, Kentucky*; <sup>3</sup>*Hepatobiology and Toxicology Center, University of Louisville, LOUISVILLE, Kentucky*; <sup>4</sup>*Department of Pharmacology and Toxicology, University of Louisville School of Medicine, Louisville, Kentucky*; <sup>5</sup>*Robley Rex Veterans Affairs Medical Center, Louisville, Kentucky*; <sup>6</sup>*Alcohol Research Center, University of Louisville, Louisville, Kentucky*

### PROTEINS: PTMS I 658-677

- WP 658 **Enrichment of Methylated Peptides Using Strong Cation Exchange with an Optimized Salt Gradient**; Amanda Ziegler<sup>1</sup>; Jessica M Conforti<sup>1</sup>; Hadden K Swany<sup>1</sup>; Charli S

## WEDNESDAY POSTERS

- WP 668 **An Integrated Multi-PTM Workflow for Simultaneous Analysis of Phosphorylation, Glycosylation, Acetylation and Ubiquitination;** Yuanwei Xu<sup>1</sup>; T. Mamie Lih<sup>2</sup>; Lijun Chen<sup>2</sup>; Hui Zhang<sup>2,3</sup>; <sup>1</sup>*Johns Hopkins University, Baltimore;* <sup>2</sup>*Johns Hopkins University School of Medicine, Baltimore city, MD;* <sup>3</sup>*Johns Hopkins University, Baltimore, MD*
- WP 669 **Mapping Post-Translational Modifications of the oncoprotein MEK1 by Tandem Top-down Proteomics;** Raveena Gupta<sup>1</sup>; Jared O Kafader<sup>1</sup>; Bryon S Drown<sup>1</sup>; Paul J Hergenrother<sup>2</sup>; Craig M Horbinski<sup>3</sup>; Neil L Kelleher<sup>1</sup>; <sup>1</sup>*Northwestern University, Evanston, IL;* <sup>2</sup>*University of Illinois Urbana-Champaign, Champaign, IL;* <sup>3</sup>*Northwestern University, Feinberg School of Medicine, Chicago, IL*
- WP 670 **Untargeted phosphoproteomics reveals unique biomarkers of colorectal cancer;** Ashima Mehta<sup>1</sup>; Adam D. Richardson<sup>1</sup>; Ethan Stancliffe<sup>1</sup>; Monil Gandhi<sup>1</sup>; Gary J. Patti<sup>1,2</sup>; <sup>1</sup>*Panome Bio, Saint Louis, MO;* <sup>2</sup>*Washington University in Saint Louis, St. Louis, MO*
- WP 671 **Mass Spectrometry Analysis of Intact Glycopeptides from Formalin-Fixed Paraffin-Embedded Prostate Tissue Samples;** Abel Bermudez<sup>1</sup>; Fernando Garcia-Marques<sup>2</sup>; Hongjian Zhao<sup>1</sup>; Dalin Zhang<sup>2</sup>; James D. Brooks<sup>2</sup>; Sharon J Pitteri<sup>2</sup>; <sup>1</sup>*Stanford University, Palo Alto, CA;* <sup>2</sup>*Stanford University, Stanford, CA*
- WP 672 **Protein search engine using databases annotated with proteoforms from UniprotKB;** Titus H Jung<sup>1</sup>; Casimir Bamberger<sup>2</sup>; Salvador Martinez De Bartolome<sup>3</sup>; Robin Park<sup>4</sup>; John R. Yates III<sup>2</sup>; <sup>1</sup>*The Scripps Research Institute, La Jolla, CA;* <sup>2</sup>*Scripps Research, La Jolla, CA;* <sup>3</sup>*Yatiri Biosciences, San Diego, CA;* <sup>4</sup>*Bruker Daltonics GmbH & Co. KG, Billerica, MA*
- WP 673 **Quantitative analysis of non-histone lysine methylation sites and lysine demethylases in breast cancer cell lines;** Christine A Berryhill<sup>1</sup>; Emma H Doud<sup>1</sup>; Amber L Mosley<sup>1</sup>; Evan M Cornett<sup>1</sup>; <sup>1</sup>*Indiana University School of Medicine, Indianapolis, IN*
- WP 674 **Structural basis for polyglutamate chain initiation and elongation by TLL family enzymes;** Kishore K Mahalingam<sup>1</sup>; Keith Keenan<sup>1</sup>; Madeleine Strickland<sup>2</sup>; Yan Li<sup>3</sup>; Yanjie Liu<sup>4</sup>; Haydn L Ball<sup>5</sup>; Martin E. Tanner<sup>4</sup>; Nico Tjandra<sup>2</sup>; Antonina Roll-Mecak<sup>1,2</sup>; <sup>1</sup>*Cell Biology and Biophysics Unit, Porter Neuroscience Research Center, National Institute of Neurological Disorders and Stroke, Bethesda, MD;* <sup>2</sup>*Biochemistry & Biophysics Center, National Heart, Lung and Blood Institute, Bethesda, MD;* <sup>3</sup>*Proteomics Core Facility, NINDS, Bethesda, MD;* <sup>4</sup>*Department of Chemistry, University of British Columbia, Vancouver, British Columbia;* <sup>5</sup>*University of Texas Southwestern Medical Center, Protein Chemistry Technology Center, Dallas, TX*
- WP 675 **Phosphoproteomics profiling reveals the kinome regulated signaling pathways in human dendritic cells treated with immunomodulators under IFN-g triggered inflammatory stress;** Cristina C Clement<sup>1</sup>; Rajesh K Soni<sup>2</sup>; Laura Santambrogio<sup>1</sup>; <sup>1</sup>*Weill Cornell Medicine, New York, NY;* <sup>2</sup>*Proteomics and Macromolecular Crystallography Shared Resource, Herbert Irving Comprehensive Cancer Center, Columbia University Irving Medical Center, New York, NY*
- WP 676 **Application of sub-unit intact mass to screen antibody chemical liabilities in early-stage discovery;** Xiaohua Liu<sup>1</sup>; Sagar Kathuria<sup>1</sup>; Nancy Yongjia Gong<sup>1,2</sup>; Zachary Beamer<sup>3</sup>; <sup>1</sup>*Sanofi, Cambridge, MA;* <sup>2</sup>*Rutgers University, New Brunswick, NJ;* <sup>3</sup>*Sanofi, Framingham, MA*
- WP 677 **Optimization and Characterization of Disulfide Linkages in the Complex Cysteine Engineered Stapled scFV for Bispecific Antibodies;** Abby J. Chiang<sup>1</sup>; Elsa Gorre<sup>2</sup>; Alexander N. Barnakov<sup>2</sup>; Christopher Sauer<sup>2</sup>; Reiko Kiyonami<sup>3</sup>; Min Du<sup>3</sup>; Andrew Mahan<sup>2</sup>; Hirsh Nanda<sup>2</sup>; <sup>1</sup>*Protein Metrics, LLC, Cupertino, CA;* <sup>2</sup>*JOHNSON AND JOHNSON, Spring House, PA;* <sup>3</sup>*Thermo Fisher Scientific, Lexington, MA*
- WP 678 **Stem cell differentiation analysis by top-down proteomics using capillary zone electrophoresis-ion mobility spectrometry-mass spectrometry;** Jorge A. Colon-Rosado<sup>1</sup>; Zhaoran Zhang<sup>1</sup>; Yuan Wang<sup>1</sup>; Liangliang Sun<sup>1</sup>; <sup>1</sup>*Michigan State University, East Lansing, MI*
- WP 679 **Residue-specific backbone cleavage of intact proteins directed by photoactive alpha radicals;** Lin He<sup>1</sup>; Ryan R. Julian<sup>1</sup>; <sup>1</sup>*University of California, Riverside, Riverside, CA*
- WP 680 **Top-down cross-linking method for analyzing in vivo quaternary structure detects the elusive heterodimer of ALS-associated SOD1 variant and wild-type SOD1;** David E. Verrill<sup>1</sup>; Katharina E. Meijboom<sup>2</sup>; Robert H Brown Jr.<sup>2</sup>; Jeffrey N. Agar<sup>1</sup>; <sup>1</sup>*Barnett Institute of Chemical and Biological Analysis, Dept. of Chemistry and Chemical Biology, Northeastern University, Boston, MA;* <sup>2</sup>*Department of Neurology, University of Massachusetts Medical School, Worcester, Massachusetts*
- WP 681 **Leveraging gas-phase fractionation and ion-ion reactions for the spatial analysis of the intact human proteome up to 70 kDa;** Jake T Kline<sup>1</sup>; Jingjing Huang<sup>2</sup>; Christopher Mullen<sup>3</sup>; Joseph B Greer<sup>4</sup>; David Bergen<sup>3</sup>; Michael W Belford<sup>3</sup>; Cornelia L Boeser<sup>3</sup>; Vlad Zabrouskov<sup>3</sup>; Kenneth R Durbin<sup>4</sup>; Graeme C McAlister<sup>3</sup>; Rafael D Melani<sup>3</sup>; Luca Fornelli<sup>1</sup>; <sup>1</sup>*University of Oklahoma, Norman, OK;* <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA;* <sup>3</sup>*Thermo Fisher Scientific – 355 River Oaks Pkwy, San Jose, California;* <sup>4</sup>*Proteinaceous, Inc., Evanston, IL*
- WP 682 **Improved Top-down Sequencing of Protein Ions via Mobility Enhanced Pseudo-MS3 Collisional Activation;** Katherine A Graham<sup>1</sup>; Nicholas B. Borotto<sup>1</sup>; <sup>1</sup>*University of Nevada Reno, Reno, NV*
- WP 683 **Unified LC-DAD-MS method for accurate and reproducible analysis of miscellaneous intact protein samples in a core facility setting;** Serge Chesnov<sup>1</sup>; Ralph Schlapbach<sup>1</sup>; Paolo Nanni<sup>1</sup>; <sup>1</sup>*Functional Genomics Center Zurich – ETH Zurich/University of Zurich, Zurich, Switzerland*
- WP 684 **Application of 210Po charge reduction to facilitate the characterization of intact proteins by 193 nm ultraviolet photodissociation;** Sean D Dunham<sup>1</sup>; Jennifer Brodbelt<sup>1</sup>; <sup>1</sup>*University of Texas at Austin, Austin, TX*
- WP 685 **Sequence Analysis of Proteins enhanced by TIMS-Enabled Next-Generation MALDI Top-Down Sequencing using a Dedicated Software Workflow;** Arndt Asperger<sup>1</sup>; Mariangela Kosmopoulou<sup>2</sup>; Dodge Baluva<sup>3</sup>; Detlev Suckau<sup>1</sup>; <sup>1</sup>*Bruker Daltonics GmbH & Co. KG, Bremen, Germany;* <sup>2</sup>*Fasmatech Science and Technology, Athens, Greece;* <sup>3</sup>*Bruker Scientific LLC, San Jose, CA*
- WP 686 **An Expanded RAS Proteoform Landscape Provided by Top-Down Analysis of Malignant Cell Lines;** Grace M. Scheidemantle<sup>1</sup>; Robert A. D'Ippolito<sup>1</sup>; Kanika Sharma<sup>1</sup>; Nicole Fer<sup>1</sup>; Brian Smith<sup>1</sup>; Mackenzie Meyer<sup>1</sup>; Scott Eury<sup>1</sup>; Abigail Neish<sup>1</sup>; Katie Powell<sup>1</sup>; Vanessa Wall<sup>1</sup>; William Burgan<sup>1</sup>; Dominic Esposito<sup>1</sup>; Anna E. Maciag<sup>1</sup>; Frank McCormick<sup>1,2</sup>; Dwight V. Nissley<sup>1</sup>; Caroline DeHart<sup>1</sup>; <sup>1</sup>*Frederick National Laboratory for Cancer Research, Frederick, MD;* <sup>2</sup>*Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA*
- WP 687 **Fast Top-Down Analysis via Orbitrap and Astral Analyzers;** Hamish Stewart<sup>1</sup>; Tabiwang Arrey<sup>1</sup>; Eugen Damoc<sup>1</sup>; Max Hoek<sup>1</sup>; Christian Hock<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Bremen, Germany*
- WP 688 **Capillary Electrophoresis-Mass Spectrometry with Cationic Polymer Coating for Reproducible Measurement of Proteoforms;** Guangyao Gao<sup>1</sup>; Qianjie Wang<sup>1</sup>; Liangliang Sun<sup>1</sup>; <sup>1</sup>*Michigan State University Department of Chemistry, East Lansing, MI*
- WP 689 **Mapping Top-Down Mass Spectrometry Data onto Three-Dimensional Protein Structures for Elucidation of Structural Proteoform Insights;** Jessie A. Bolger<sup>1</sup>; Kenneth R. Durbin<sup>1</sup>; Matthew T. Robey<sup>1</sup>; Ryan T. Fellers<sup>1,2</sup>; <sup>1</sup>*Proteinaceous, Evanston, IL;* <sup>2</sup>*Northwestern University, Evanston, IL*

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- WP 690 **The Development of Optimized Cyclic Ion Mobility-Mass Spectrometry Methods for Native Top-Down Proteomics;** Ryan K Schroeder<sup>1</sup>; Devin Makey<sup>1</sup>; Carolina Rojas Ramirez<sup>2</sup>; Brandon T Ruotolo<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Michigan, Ann Arbor, Michigan; <sup>2</sup>Department of Pathology, University of Michigan, Ann Arbor, Michigan 48109, United States, Ann Arbor, Michigan
- WP 691 **In-Depth Characterization of Protein Kinase Complexes by Top-Down Mass Spectrometry;** Hsin-Ju Chan<sup>1</sup>; Boris Krichel<sup>2</sup>; Emily A. Reasoner<sup>1</sup>; Man-Di Wang<sup>1</sup>; Ying Ge<sup>1,2,3</sup>; <sup>1</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Cell and Regenerative Biology, Madison, WI; <sup>3</sup>Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI
- WP 692 **Multidimensional Sample Pre-Fractionation Workflow for Deep Middle-Down Proteomics;** Ayako Takemori<sup>1</sup>; Philipp T. Kaulich<sup>2</sup>; Andreas Tholey<sup>2</sup>; Nobuaki Takemori<sup>1</sup>; <sup>1</sup>Ehime University, Toon, Japan; <sup>2</sup>Christian-Albrechts-Universität zu Kiel, Kiel, Germany
- WP 693 **FLASHViewer: a web application with a configurable layout for top-down mass spectrometry data visualization;** Jihyung Kim<sup>1,2</sup>; Andrew Almaguez<sup>3</sup>; Kyowon Jeong<sup>1,2</sup>; Jaekwan Kim<sup>4</sup>; Axel Walter<sup>1,2</sup>; Wonhyeuk Jeong<sup>5</sup>; Oliver Kohlbacher<sup>1,2,6</sup>; <sup>1</sup>University of Tübingen, Tübingen, Germany; <sup>2</sup>Institute for Bioinformatics and Medical Informatics, University of Tübingen, Tübingen, Germany; <sup>3</sup>Jambit GmbH, Stuttgart, Germany; <sup>4</sup>Omics Research Center, Sejong, South Korea; <sup>5</sup>Yale School of Medicine, New Haven, CT; <sup>6</sup>Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany
- WP 694 **FLASHIda:FAIMS - Intelligent Data Acquisition for FAIMS enabled Top-Down Proteomics;** Tom D. Müller<sup>1,2</sup>; Kyowon Jeong<sup>1,2</sup>; Philipp T. Kaulich<sup>3</sup>; Andreas Tholey<sup>3</sup>; Oliver Kohlbacher<sup>1,2,4</sup>; <sup>1</sup>Applied Bioinformatics, Department for Computer Science, University of Tübingen, Tübingen, Germany; <sup>2</sup>Institute for Bioinformatics and Medical Informatics, University of Tübingen, Tübingen, Germany; <sup>3</sup>Systematic Proteome Research & Bioanalytics, Institute for Experimental Medicine, Christian-Albrechts-Universität zu Kiel, Kiel, Germany; <sup>4</sup>Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany
- WP 695 **Top-Down Protein Sequencing of Simple Protein Mixtures combining Liquid Chromatography and Cyclic Ion Mobility TOF Mass Spectrometry;** Marie LEY<sup>1</sup>; Victor COCHARD<sup>1</sup>; Véronique LEGROS<sup>1</sup>; Jean-Michel CAMADRO<sup>1</sup>; Guillaume CHEVREUX<sup>1</sup>; <sup>1</sup>ProteoSeine CNRS, Institut Jacques Monod, Université Paris Cité, Paris, France
- WP 696 **Probing Non-Covalent Interactions Between Proteins and Small Molecules with Photoactivated Radical Dissociation;** Evan E Hubbard<sup>1</sup>; Ryan R. Julian<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- WP 697 **Improved top-down analysis of antibody subunits using the Omnitrap-Orbitrap-Booster platform;** Camille Garcia<sup>1,2,3</sup>; Konstantin O. Nagornov<sup>4</sup>; Athanasios Smyrnakis<sup>5</sup>; Anton N. Kozhinov<sup>4</sup>; Dimitris Papanastasiou<sup>5</sup>; Yury O. Tsybin<sup>4,6</sup>; Julia Chamot-Rooke<sup>1</sup>; <sup>1</sup>Institut Pasteur, Paris, France; <sup>2</sup>Université Paris Cité, Paris, France; <sup>3</sup>CNRS UAR2024, Paris, France; <sup>4</sup>Spectroswiss, Lausanne, Switzerland; <sup>5</sup>Fasmatech, Athens, Greece; <sup>6</sup>Spectrotech, Lyon, France
- WP 698 **Native Mass Spectrometry and Top-Down MS of Acyl-Lysine Modified Protein Complexes;** Yi Qiao<sup>1</sup>; Boyu Zhao<sup>1</sup>; Rachel Loo<sup>2</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>University of California, Los Angeles, Los Angeles, CA; <sup>2</sup>University of California Los Angeles, Los Angeles, CA
- WP 699 **Top-down proteomics analysis of pg-level cell lysate using spray-capillary CE-FAIMS-MS;** Samin Anjum<sup>1</sup>; Zhitao Zhao<sup>2</sup>; Kellye A Cupp-Sutton<sup>1</sup>; Si Wu<sup>1</sup>; <sup>1</sup>The University of Alabama, Tuscaloosa, AL; <sup>2</sup>University of Oklahoma, Norman, OK
- WP 700 **Revealing Cerezyme Glycoforms by Native Capillary Zone Electrophoresis Mass Spectrometry (nCZE-MS);** Danye Qiu<sup>1</sup>; Hucong Jiang<sup>1</sup>; Tongdan Wang<sup>1</sup>; Jincui Huang<sup>1</sup>; <sup>1</sup>WuXi Biologics, Shanghai, China
- WP 701 **Advanced Top-Down Data Analysis with MetaMorpheus;** Nicholas Bollis<sup>1</sup>; Katherine B Henke<sup>2</sup>; Michael R Shortreed<sup>3</sup>; Lloyd M Smith<sup>3</sup>; <sup>1</sup>University of Wisconsin Madison, Madison, WI; <sup>2</sup>Yale School of Medicine, New Haven, CT; <sup>3</sup>University of Wisconsin-Madison, Madison, WI
- WP 702 **Enhancing Top-Down Mass Spectrometry Intact Protein Characterization through Aggregation of Multimodal Fragmentation Data;** Ken Durbin<sup>1</sup>; Matthew T. Robey<sup>2</sup>; Ryan T. Fellers<sup>2</sup>; Joseph B. Greer<sup>2</sup>; Bryan P. Early<sup>2</sup>; Daisha Utley<sup>2</sup>; <sup>1</sup>Proteinaceous, Evanston, IL; <sup>2</sup>Proteinaceous, Inc., Evanston, IL
- WP 703 **Top-down Proteomics to Monitor Post-translational Protein Arginylation in Cell Systems;** Zongtao Lin<sup>1</sup>; Richard M Searfoss<sup>1</sup>; Xingyu Liu<sup>1</sup>; Axe Xie<sup>1</sup>; Emily Zahn<sup>1</sup>; Joanna M Gongora<sup>1</sup>; Rashmi Karki<sup>1</sup>; Bibhuti Bhusana Palai<sup>1</sup>; Daniel Ramirez<sup>1</sup>; Benjamin Garcia<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO
- WP 704 **Combining Top-Down and Bottom-Up Mass Spectrometry Paves the Way for High Throughput Polyclonal Antibody Sequencing;** Lei Xin<sup>1</sup>; Baozhen Shan<sup>1</sup>; Chao Peng<sup>2</sup>; Jun Ma<sup>2</sup>; Shuyang Zhang<sup>1</sup>; Zihao Wang<sup>1</sup>; Wenting Li<sup>1</sup>; <sup>1</sup>Bioinformatics Solutions Inc., Waterloo, ON; <sup>2</sup>BaizhenBio Inc., Wuhan, China
- WP 705 **Capillary Zone Electrophoresis-Mass Spectrometry Reveals Histone Modification Patterns Change in Isogenic SW480 and SW620 Cell Lines;** Fei Fang<sup>1</sup>; Brian D Fries<sup>2</sup>; Amanda Hummons<sup>2</sup>; Liangliang Sun<sup>1</sup>; <sup>1</sup>Department of Chemistry, Michigan State University, East Lansing, MI; <sup>2</sup>Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH
- WP 706 **Introducing FRAGMAPS Software: a One-stop Shop for Internal Fragment Analysis With Multi-Level Disambiguation, Intensity-based Visualization, Quantification, and Inter-sample Comparison;** Novera Alam<sup>1</sup>; Somak Ray<sup>1</sup>; Jeffrey N. Agar<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA
- WP 707 **Benchmarking A Visual Acuity Ion Classifier for MS/MS Deconvolution and Identification of Native Membrane Proteins In Vitro;** Adrian L Guthals<sup>1</sup>; Wonhyeuk Jung<sup>2</sup>; Aniruddha Panda<sup>2</sup>; Blake Hakkila<sup>1</sup>; Stephanie Sturgeon<sup>1</sup>; Timothy Djang<sup>3</sup>; Alex Gavrilenko<sup>4</sup>; Jhenya Gavrilenko<sup>4</sup>; Panos Iatrou<sup>4</sup>; Stelios Gkegkas<sup>4</sup>; Derrill Sturgeon<sup>4</sup>; Rachel Franklin<sup>1</sup>; Yury V. Vasilev<sup>1</sup>; Diana Oppenheimer<sup>1</sup>; Joseph Meeuswen<sup>1</sup>; Joseph Beckman<sup>5</sup>; Kallol Gupta<sup>2</sup>; <sup>1</sup>Agilent Technologies, Corvallis, Oregon; <sup>2</sup>Yale School of Medicine, New Haven, CT; <sup>3</sup>Agilent Technologies, Santa Clara, CA; <sup>4</sup>Devicepros, Boston, USA, MA; <sup>5</sup>Oregon State University, Corvallis
- WP 708 **Improving the top-down sequencing of disulfide-bonded proteins by leveraging multiple ion activation techniques in both positive and negative ionization modes;** Cynthia N. Nagy<sup>1</sup>; Ruben Szabo<sup>2</sup>; Kenneth R. Durbin<sup>3</sup>; Luca Fornelli<sup>1</sup>; <sup>1</sup>University of Oklahoma, Norman, OK; <sup>2</sup>University of Debrecen, Debrecen, Hungary; <sup>3</sup>Proteinaceous, Inc., Evanston, IL

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- WP 709 **Variance from sequential multi-omic extractions impact biological interpretation of viral disease model;** Molly Soper-Hopper<sup>1</sup>; Colt Capan<sup>1</sup>; Hyuongjoo Lee<sup>1</sup>; Ryan D Sheldon<sup>1</sup>; <sup>1</sup>Van Andel Institute, Grand Rapids, MI
- WP 710 **Complementary ion quantification enables accurate multiplexing on the Orbitrap Astral;** Alex Johnson<sup>1</sup>; Martin Zeller<sup>2</sup>; Hamish Stewart<sup>2</sup>; Graeme McAlister<sup>3</sup>; Martin Wühr<sup>1</sup>; <sup>1</sup>Princeton University, Princeton, NJ; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>ThermoFisher Scientific, San Jose, CA
- WP 711 **Proteomelit 1.0: User-friendly and comprehensive software package for MS-based proteomics data analysis;** Ana Rita Colaco<sup>1</sup>; David Oliver Schlessinger<sup>1</sup>; Michael Wierer<sup>1</sup>; <sup>1</sup>Proteomics Research Infrastructure, Novo

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- WP 712 **Nascent proteomics reveals divergent contributions of 40 translation initiation factors to shaping the proteome;** Toman Bortecen<sup>1,2</sup>; Robert Kalis<sup>3</sup>; Johannes Zuber<sup>3</sup>; Jeroen Krijgsveld<sup>1, 4</sup>; <sup>1</sup>German Cancer Research Center (DKFZ), Heidelberg, Germany; <sup>2</sup>Heidelberg University, Heidelberg, Germany; <sup>3</sup>Institute of Molecular Pathology (IMP), Vienna, Austria; <sup>4</sup>Heidelberg University, Medical Faculty, Heidelberg, Germany
- WP 713 **Melanoma cells develop vemurafenib resistance through epitranscriptomic regulation;** Shiyuan Guo<sup>1</sup>; Tianyu F. Qi<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- WP 714 **Understanding early proteomic response of *Saccharomyces cerevisiae* to different oxidants using label-free comparative proteomics analysis;** Debasish Ghosh<sup>1</sup>; Khadiza Zaman<sup>2</sup>; Laszlo Prokai<sup>2</sup>; Vladimir Shulaev<sup>1</sup>; <sup>1</sup>UNIVERSITY OF NORTH TEXAS, Denton, TX; <sup>2</sup>University of North Texas Health Science Center, Department of Pharmacology and Neuroscience, Fort Worth, Texas
- WP 715 **A Proteome-wide Comparison of TMT-based and DIA-based Datasets Using the Orbitrap Astral Mass Spectrometer;** Yuchen He<sup>1</sup>; Joao A. Paulo<sup>1</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup>Harvard Medical School, Boston, MA
- WP 716 **Species-deconvolved proteomics enables accurate identification and quantification of cancer and stromal proteins in patient-derived xenografts;** Shuo Qian<sup>1</sup>; Han Liu<sup>2</sup>; Shichen Shen<sup>2</sup>; Jun Qu<sup>1, 2</sup>; <sup>1</sup>Roswell Park Comprehensive Cancer Center, Buffalo, NY; <sup>2</sup>SUNY at Buffalo, Buffalo, NY
- WP 717 **A multi-year longitudinal harmonization of quality controls in mass spectrometry proteomics core facilities;** Cristina Chiva<sup>1,2</sup>; Roger Olivella<sup>1,2</sup>; An Staes<sup>3,4,5</sup>; Teresa Mendes Maia<sup>3,4,5</sup>; Francis Impens<sup>3,4,5</sup>; Simon Devos<sup>3,4,5</sup>; Christian Panse<sup>6,7</sup>; Karel Stejskal<sup>8,9,10</sup>; Karl Mechtler<sup>8,9,10</sup>; Thibaut Douché<sup>11</sup>; Mariette Matondo<sup>11</sup>; Bérandère Lombard<sup>12</sup>; Damarys Loew<sup>12</sup>; Mandy Rettel<sup>13</sup>; Dominic Helm<sup>13,14</sup>; Andrea Schuhmann<sup>15</sup>; Anna Shevchenko<sup>15</sup>; Paolo Nanni<sup>6</sup>; Eduard Sabido<sup>1,2</sup>; <sup>1</sup>Centre de Regulació Genòmica, Barcelona Institute of Science and Technology (BIST), Barcelona, Spain; <sup>2</sup>Univeritat Pompeu Fabra, Barcelona, Spain; <sup>3</sup>VIB Proteomics Core, Ghent, Belgium; <sup>4</sup>VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; <sup>5</sup>Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; <sup>6</sup>Functional Genomics Center Zurich ETHZ/UZH, Zürich, Switzerland; <sup>7</sup>Swiss Institute of Bioinformatics (SIB), Lausanne, Switzerland; <sup>8</sup>Research Institute of Molecular Pathology (IMP), Vienna Biocenter (VBC), Vienna, Austria; <sup>9</sup>IMBA Institute of Molecular Biotechnology of the Austrian Academy of Sciences, Vienna Biocenter (VBC), Vienna, Austria; <sup>10</sup>Gregor Mendel Institute (GMI), Austrian Academy of Sciences, Vienna BioCenter 7 (VBC, Vienna, Austria; <sup>11</sup>. Institut Pasteur, Université Paris Cité, Proteomics Platform, Mass Spectrometry for Biology Unit, Paris, France; <sup>12</sup>Institut Curie, PSL Research University, Centre de Recherche, CurieCoreTech Mass Spectrometry Proteomics, Paris, France; <sup>13</sup>Proteomics Core Facility, European Molecular Biology Laboratory, Heidelberg, Germany; <sup>14</sup>Proteomics Core Facility, German Cancer Research Center (DKFZ), Heidelberg, Germany; <sup>15</sup>Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany
- WP 718 **Comparing gas phase enabled spectral library generation and library free DIA based phosphoproteomics;** Dongmei Zhang<sup>1</sup>; Ling Li<sup>1</sup>; Belinda Willard<sup>1</sup>; <sup>1</sup>Cleveland Clinic, Cleveland, OH
- WP 719 **Low-input Proteomic Analysis Unveils Critical Pathways Underlying the Role of IL-4 and/or IL-13 on Human Mast Cells;** Bo Yang<sup>1</sup>; Kai-Ting Shade<sup>1</sup>; Preeti Bais<sup>1</sup>; Alexandra Hicks<sup>1</sup>; Hendrik Wesseling<sup>1</sup>; Bailin Zhang<sup>1</sup>; <sup>1</sup>Sanofi, Cambridge, MA
- WP 720 **Dynamic TRPV2 ion channel proximity proteomics links calcium flux to cellular adhesion factors NCAM and L1CAM in neurite outgrowth;** Robyn J. Eisert<sup>1</sup>; Pamela Gallo<sup>2</sup>; Elaine Mihelca<sup>2</sup>; Gary A. Bradshaw<sup>1</sup>; Marian Kalocsay<sup>3</sup>; Vera Moiseenkova-Bell<sup>2</sup>; <sup>1</sup>Harvard Medical School, Boston, MA; <sup>2</sup>University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; <sup>3</sup>MD Anderson Cancer Center, Houston, Texas
- WP 721 **Profiling of Aging-induced Proteome Alternation in Calbindin- and Calretinin-positive Neurons in Mouse Hippocampus with a microPOTS Platform;** Yen-Chen Liao<sup>1</sup>; Jeong Han Lee<sup>2</sup>; Sarah M Williams<sup>1</sup>; Lisa M Bramer<sup>2</sup>; Ljiljana Paša-Tolić<sup>1</sup>; Ying Zhu<sup>1</sup>; Ebenezer N. Yamoah<sup>2</sup>; <sup>1</sup>Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Department of Physiology and Cell Biology, School of Medicine, University of Nevada, Reno, NV; <sup>3</sup>Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA
- WP 722 **High-resolution MS1 ion-current-based quantification combined with deconvolution of chimeric MS2 spectra enables in-depth quantitative proteomics and application in spatial proteomics;** Shuo Qian<sup>1</sup>; Shichen Shen<sup>2</sup>; Shihan Huo<sup>2</sup>; Min Ma<sup>1</sup>; Sailee Rasam<sup>2</sup>; Jun Qu<sup>1, 2</sup>; <sup>1</sup>Roswell Park Comprehensive Cancer Center, Buffalo, NY; <sup>2</sup>SUNY at Buffalo, Buffalo, NY
- WP 723 **Deciphering Molecular mechanisms: Neuropeptide Signaling Pathways Explored Through Proteomic Analysis in Rat brain tissue;** Meera Asokan<sup>1</sup>; Abby Askins<sup>2</sup>; Luis Natividad<sup>2</sup>; <sup>1</sup>University of Texas Austin, Austin, TX; <sup>2</sup>University of Texas at Austin, Austin, Texas
- WP 724 **Proximity labeling together with LC-MS/MS for interrogating the proximity proteome of METTL1;** Zhongwen Cao<sup>1</sup>; Xingyuan Chen<sup>1</sup>; Quanqing Zhang<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- WP 725 **Label-Free Quantitation with High Accuracy and Precision on a Single-Cell Scale with Orbitrap Astral Mass Spectrometer: An Inter-laboratory Study;** Anna Pashkova<sup>1</sup>; Jenny Ho<sup>2</sup>; Tabiwang N. Arrey<sup>1</sup>; Florian Marty<sup>3</sup>; Eugen Damoc<sup>1</sup>; Min Huang<sup>4</sup>; Sonja Radau<sup>5</sup>; Shio Watanabe<sup>6</sup>; Pedro Navarro<sup>7</sup>; <sup>1</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; <sup>3</sup>Thermo Fisher Scientific, Reinach, Switzerland; <sup>4</sup>Thermo Fisher Scientific, Shanghai, China; <sup>5</sup>Thermo Fisher Scientific, Dreieich, Germany; <sup>6</sup>Thermo Fisher Scientific, Yokohama, Japan; <sup>7</sup>Thermo Fisher Scientific, Bremen, Germany
- WP 726 **Harmonization of sample preparation and acquisition methods enables world-wide method transfer of proteomics workflows;** Jan Muntel<sup>1</sup>; Sandra Schär<sup>2</sup>; Luca Raess<sup>2</sup>; Christopher Below<sup>2</sup>; Roland Bruderer<sup>2</sup>; Jakob Vowinkel<sup>2</sup>; Nigel Beaton<sup>1</sup>; <sup>1</sup>Biognosys Inc, Newton, MA; <sup>2</sup>Biognosys AG, Schlieren, Switzerland
- WP 727 **Deciphering the Proteomic Molecular Signatures of Traumatic Brain Injury in Serum and CSF by LC-MS/MS;** Vishal Sandilya<sup>1</sup>; Mojgan Atashi<sup>1</sup>; Thu Nguyen<sup>1</sup>; Joy O Solomon<sup>1</sup>; Md Mostofa Al Amin Bhuiyan<sup>1</sup>; Cristian D Gutierrez-Reyes<sup>1</sup>; Waziha Tasnim Purba<sup>1</sup>; Mojibola Fowowe<sup>1</sup>; Judith Ijeoma Nwaiwu<sup>1</sup>; Firas Kobeissy<sup>2</sup>; Stefania Mondello<sup>3</sup>; Ava M Puccio<sup>4</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, Texas; <sup>2</sup>Morehouse School of Medicine, Atlanta, Georgia; <sup>3</sup>University of Messina, Messina, Italy; <sup>4</sup>University of Pittsburgh, Pittsburgh, PA
- WP 728 **Use targeted proteomics analysis of key pathways to optimize cell culture media and feeds for Chinese Hamster Ovary cells;** Km Shams Ud Doha<sup>1</sup>; Martin Ciganda<sup>1</sup>; Chengjian Tu<sup>1</sup>; Didar Asik<sup>1</sup>; Jaime S Goldfuss<sup>1</sup>; Scott Jacobia<sup>1</sup>; Andy M Campbell<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Grand Island, NY
- WP 729 **Double Immunoprecipitation (dIP) Trapping and Proteomics Mass Spectrometry to Discover Substrates of HDAC1 Involved in Sick Cell Anemia;** Eric T.J Davis<sup>1</sup>;

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- Urvashi Thongam<sup>2</sup>; Jennell White<sup>2</sup>; Mary K H Pflum<sup>2</sup>; <sup>1</sup>Wayne State University, Detroit, MI; <sup>2</sup>Wayne State University, Detroit, MI
- WP 730 **A semi-automated SP3 sample preparation method for high throughput screening of in vivo BiLD labeling on an Orbitrap Astral**; Greg Waitt<sup>1</sup>; Jaebin Kim<sup>2</sup>; Lucio Schiapparelli<sup>2</sup>; Scott Soderling<sup>2</sup>; Erik Soderblom<sup>1, 2</sup>; <sup>1</sup>Proteomics and Metabolomics Core Facility, Duke University School of Medicine, Durham, NC; <sup>2</sup>Department of Cell Biology, Duke University School of Medicine, Durham, NC
- WP 731 **Evaluation of different lysine specific peptidases for MS-based proteomics**; Tanveer Singh Bath<sup>1</sup>; Cristina Hernandez Rollan<sup>1</sup>; Morten Nørholm<sup>2</sup>; Jesper Velgaard Olsen<sup>1</sup>; <sup>1</sup>Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark; <sup>2</sup>NNF Center for Biosustainability, Denmark Technical University, Lyngby, Denmark
- WP 732 **Evaluation and optimization of FAIMS-based gas phase fractionation for increased DIA spectral library coverage on an Orbitrap Astral**; Tricia Ho<sup>1</sup>; Erik Soderblom<sup>1</sup>; <sup>1</sup>Proteomics and Metabolomics Core Facility, Duke University School of Medicine, Durham, NC
- WP 733 **Expanding TMTpro reagents to 32-plex for high-throughput quantitative proteomics on Orbitrap platforms**; Dustin Frost<sup>1</sup>; Joao A. Paulo<sup>2</sup>; Steven P. Gygi<sup>2</sup>; Karsten Kuhn<sup>3</sup>; Ian Pike<sup>3</sup>; Ryan Bomgarden<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Rockford, Illinois; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>Proteome Sciences, London, United Kingdom
- WP 734 **Toward Global Estimation of Endoplasmic Reticulum Import Efficiency via Sec61 Blockade and Proximity Labeling Mass Spectrometry**; Ziqi Lyu<sup>1</sup>; Joseph C. Genereux<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- WP 735 **Protein identification and quantitation using scanning data-independent acquisition (DIA)**; Wen Jin<sup>1</sup>; Leroi DeSouza<sup>1</sup>; Alina Dindyal-Popescu<sup>1</sup>; Doug Simmons<sup>1</sup>; <sup>1</sup>SCIEX, Concord, ON
- WP 736 **Exploring Drought Tolerance: Comparative Proteomics of Different Brassica rapa Plant Genotypes Using LFQ**; Brandon Anselmo Saiz<sup>1</sup>; Benjamin Conrad Romanjenko<sup>1</sup>; Carmela Rosaria Guadagno<sup>1</sup>; Brent E. Ewers<sup>1</sup>; Franco Basile<sup>1</sup>; <sup>1</sup>University of Wyoming, Laramie, WY
- WP 737 **Applications and characterization of a new deuterium-enhanced TMTpro 32-plex reagent set for sample multiplexing**; Nathan Zuniga<sup>1</sup>; Dustin Frost<sup>2</sup>; Karsten Kuhn<sup>3</sup>; Ryan Bomgarden<sup>2</sup>; Ian Pike<sup>3</sup>; Steven P. Gygi<sup>1</sup>; Joao A. Paulo<sup>1</sup>; <sup>1</sup>Harvard Medical School, Boston, MA; <sup>2</sup>Thermo Fisher Scientific, Bannockburn, IL; <sup>3</sup>Proteome Sciences, London, United Kingdom
- WP 738 **An in-depth investigation into plasma proteomic studies using DIA mass spectrometry and affinity-based platforms**; Aron Phong<sup>1</sup>; Balazs Szoke<sup>1</sup>; Benoit Lehallier<sup>1</sup>; Scott Lohr<sup>1</sup>; Sara Ahadi<sup>1</sup>; <sup>1</sup>Alkermest Inc., San Carlos, CA
- WP 739 **Exploring whether Retrotranslocation During ER-Associated Protein Degradation is Affected by Proteasome Inhibition**; Qiqi Lin<sup>1</sup>; Ziqi Lyu<sup>1</sup>; Jasmine Castellanos<sup>1</sup>; Joseph Genereux<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- WP 740 **Quantitative proteomic analysis of the protein levels involved in the maturation of the mammalian oocytes**; Piotr Suder<sup>1</sup>; Paulina Kret<sup>1</sup>; Wieslawa Mlodawska<sup>2</sup>; Igor Kotsan<sup>1</sup>; Anna Bodzon-Kulakowska<sup>1</sup>; <sup>1</sup>AGH University of Krakow, Krakow, Poland; <sup>2</sup>University of Agriculture, Cracow, Poland
- WP 741 **Label-free quantitative proteomic analysis of spinal cord after morphine treatment**; Przemyslaw Mielczarek<sup>1, 2</sup>; Anna Bodzon-Kulakowska<sup>3</sup>; Jolanta H. Kotlinska<sup>4</sup>; Jerzy Silberring<sup>3</sup>; <sup>1</sup>AGH University, Krakow, Poland; <sup>2</sup>Polish Academy of Sciences, Krakow, Poland; <sup>3</sup>AGH University of Krakow, Krakow, Poland; <sup>4</sup>Medical University of Lublin, Lublin, Poland
- WP 742 **Comparative proteome quantification reveals novellongevity regulators in IIS pathway of C. elegans**; LANG DING; Baylor College of Medicine, Houston, TX
- WP 743 **Protein Mistargeting Triggers a Cytosolic Quality Control Mechanism that Sorts Proteins Based on Thermodynamic Stability**; Jasmine Castellanos<sup>1</sup>; Joseph Genereux<sup>2</sup>; Khanh Nguyen<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA; <sup>2</sup>University of California Riverside, Riverside, CA

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- WP 744 **Investigating Proteomic Changes Induced by Young Plasma Transfusion in the Recovery of Traumatic Brain Injury in Mice**; Wen-Chen Chen<sup>1</sup>; Wei-Che Chang<sup>1</sup>; Hsiao-Wei Chen<sup>1</sup>; Guo-Jen Huang<sup>1</sup>; Yi-Ting Chen<sup>1</sup>; <sup>1</sup>Chang Gung Memorial University, Tao-yuan City, Taiwan
- WP 745 **Deep Lung Proteome Analysis of Bronchopulmonary Dysplasia Using TMS TOF Ultra and 480 Explorer**; Daniela M Schlatter<sup>1</sup>; Mark R Chance<sup>1</sup>; Anantha Krishnan Harijith<sup>1, 2</sup>; Filipa Blasco Tavares Pereira Lopes<sup>1</sup>; Tara Sudhadevi<sup>1</sup>; Matthew Willetts<sup>3</sup>; Diego Assis<sup>3</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>University Hospitals, Cleveland, OH; <sup>3</sup>Bruker Daltonics, Billerica, MA
- WP 746 **Proteomic Stability in Archival Formalin-Fixed and Paraffin-Embedded (FFPE) Tissue Sections Stored on Glass Slides by Mass Spectrometry**; Anqi Tu<sup>1</sup>; Beom-Jun Kim<sup>1</sup>; Nicolas Giraldo<sup>1</sup>; Chris Richardson<sup>1</sup>; David Chain<sup>1</sup>; Steve Sweet<sup>1</sup>; Yeoun Jin Kim<sup>1</sup>; Andrew Chambers<sup>1</sup>; <sup>1</sup>AstraZeneca, Gaithersburg, MD
- WP 747 **iCAB: an insitu cell-type specific proteome analysis method using antibody-mediated biotinylation**; Taekyung Ryu<sup>1</sup>; Seok-Young Kim<sup>1</sup>; Thujitha Thuraisamy<sup>1</sup>; Jisu Shin<sup>1</sup>; Yura Jang<sup>1</sup>; Tae-In Kam<sup>1, 2</sup>; Chan-Hyun Na<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD; <sup>2</sup>Korea Advanced Institute of Science and Technology, Daejeon, South Korea
- WP 748 **Pushing the limits of deep proteome analysis in muscle tissue**; Bingnan Zhao<sup>1</sup>; Noah M Lancaster<sup>1, 2</sup>; Katherine A Overmyer<sup>1, 3, 4</sup>; Perla Geara<sup>5</sup>; Jeffrey F. Dilworth<sup>5</sup>; Joshua J Coon<sup>1, 2, 3, 4</sup>; <sup>1</sup>Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>Morgridge Institute for Research, Madison, WI; <sup>4</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI; <sup>5</sup>Department of Cell and Regenerative Biology, Madison, WI
- WP 749 **Molecular Profiling of KCNT1 Mouse Model with ASO Treatment**; Fangxu Sun<sup>1</sup>; Fergal Casey<sup>1</sup>; Sijia Wu<sup>1</sup>; Yuqing Liu<sup>1</sup>; Thomas Carlile<sup>1</sup>; Paymaan Jafar-nejad<sup>2</sup>; Jing Wu<sup>3</sup>; Imran Quraishi<sup>3</sup>; Maysam Pedram<sup>3</sup>; Leonard K. Kaczmarek<sup>3</sup>; Viet Nguyen<sup>1</sup>; <sup>1</sup>Biogen, Cambridge, MA; <sup>2</sup>Ionis Pharmaceuticals, Inc., Carlsbad, CA; <sup>3</sup>Yale University, New Haven, CT
- WP 750 **Laser Ablation Sampling for Formalin Fixed Paraffin Embedded Mouse Lung Tissue Proteomics**; Blessing Chisom Egbelogu<sup>1</sup>; Come J. Thieulent<sup>1</sup>; Mariano Carossino<sup>1</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA
- WP 751 **Profiling Protein-Protein Interactions in the Human Brain by Refined Co-Fractionation Mass Spectrometry**; Dong-Geun Lee<sup>1</sup>; Him Shrestha<sup>1</sup>; Junmin Peng<sup>1</sup>; <sup>1</sup>St.Jude Children's Research Hospital, Memphis, TN
- WP 752 **Proteome changes during skin wound healing in healthy humans of different ages**; Alexey Lyashkov<sup>1</sup>; Ceereena Ubaida-Mohien<sup>1</sup>; Linda Zukley<sup>1</sup>; Shepherd H. Schurman<sup>1</sup>; Mary Kaileh<sup>1</sup>; Arsun Bektas<sup>1</sup>; Yevgeniya Lukyanenko<sup>1</sup>; Ruin Moaddel<sup>1</sup>; Julián Candia<sup>1</sup>; Chee Chia<sup>1</sup>; <sup>1</sup>NIA/NIH, Baltimore, MD
- WP 753 **Ageing Signatures Analyzing Human Lung Tissues Across the Lifespan by Data-Independent Acquisition: from Infancy to the Elderly**; Jacob Rose<sup>1</sup>; Joanna Bons<sup>1</sup>; Delphine Beaulieu<sup>2</sup>; Mark Watson<sup>1</sup>; John Sembrat<sup>2</sup>; Oliver Eickelberg<sup>2</sup>; Melanie Koenigshoff<sup>2</sup>; Birgit Schilling<sup>1</sup>; <sup>1</sup>Buck



WEDNESDAY POSTERS

- Institute for Research on Aging, Novato, CA; <sup>2</sup>Center for Lung Aging and Regeneration, Division of Pulmonary Allergy Critical Care and Sleep Medicine, University of Pittsburgh, Pittsburgh, PA
- WP 754 **Rapid tissue proteome profiling with trapped ion mobility mass spectrometry;** Felix Rudolf Schneidmadel<sup>1</sup>; Denys Oliinyk<sup>1</sup>; Andreas Will<sup>1</sup>; Phillip Köcher<sup>1</sup>; Florian Meier-Rosar<sup>1</sup>; <sup>1</sup>Uniklinikum Jena, Functional Proteomics, Friedrich-Schiller-Universität, Jena, Germany
- WP 755 **Azo-Enabled Extracellular Matrix Proteomics for High-throughput Quantitative Analysis of Lung Tissue;** Anna G Towler<sup>1</sup>; Yanlong Zhu<sup>2</sup>; Timothy Aballo<sup>3</sup>; Kevin Buck<sup>4</sup>; Elizabeth Bayne<sup>4</sup>; Vanessa Morales-Tirado<sup>5</sup>; Yupeng (David) He<sup>6</sup>; Yu Tian<sup>5</sup>; Ying Ge<sup>3,4</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>Department of Cell and Regenerative Biology, Madison, WI; <sup>4</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>5</sup>AbbVie Inc., Worcester, MA; <sup>6</sup>AbbVie Inc., North Chicago, IL
- WP 756 **Automated high-throughput proteomic analysis of stored blood cells from a large cohort of non-domestic felids;** Kevin L Schauer<sup>1</sup>; Kevin Yang<sup>1</sup>; Amirmansoor Hakimi<sup>1</sup>; Eugen Damoc<sup>2</sup>; Lily AB Parkinson<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Brookfield Zoo, Chicago Zoological Society, Brookfield, IL
- WP 757 **In situ, cell-type-specific proteome analysis using antibody-mediated biotinylation in mouse midbrains with Parkinson's disease;** Taekyung Ryu<sup>1</sup>; Seok-Young Kim<sup>1</sup>; Jae-Jin Song<sup>1</sup>; Tae-In Kam<sup>1,2</sup>; Chan-Hyun Na<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD; <sup>2</sup>Korea Advanced Institute of Science and Technology, Daejeon, South Korea
- WP 758 **Characterizing Rat Placental/Amniotic Fluid Proteome: Toward Discovery of Placental Opioid Enhancing Factor (POEF) by Gel Electrophoresis and Bottom-up Proteomics;** Troy D Wood<sup>1</sup>; Brynn Nelson<sup>1</sup>; Alexandra Izydorczak<sup>1</sup>; Howell Phillips<sup>1</sup>; Jean DiPirro<sup>2</sup>; Mark Kristal<sup>1</sup>; Alexis Thompson<sup>1</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY; <sup>2</sup>Buffalo State University, Buffalo, NY
- WP 759 **Investigating ischemia and reperfusion-induced organ damage in severe cardiac arrest: A Comprehensive proteomics perspective;** Ju Yeon Lee<sup>1, 2</sup>; Muhammad Shoaib<sup>3</sup>; Jin-Woong Choi<sup>4</sup>; Jong Hwan Shin<sup>4</sup>; Rishabh C Choudhary<sup>5</sup>; Kei Hayashida<sup>5</sup>; Seunguk J Baek<sup>6</sup>; Santiago Miyara<sup>5</sup>; Jaewoo Choi<sup>7</sup>; Lance B Becker<sup>3, 5, 8</sup>; Junhwan Kim<sup>3, 5, 8</sup>; <sup>1</sup>Korea Basic Science Institute, Cheongju, South Korea; <sup>2</sup>University of Science and Technology, Daejeon, South Korea; <sup>3</sup>Donald and Barbara Zucker School of Medicine, Hempstead, New York; <sup>4</sup>Korea Basic Science Institute, Cheongju, South Korea; <sup>5</sup>Feinstein Institute for Medical Research, Manhasset, New York; <sup>6</sup>Johns Hopkins University, Baltimore, MD; <sup>7</sup>Oregon State University, Corvallis, Oregon; <sup>8</sup>North Shore University Hospital, Manhasset, New York
- WP 760 **dia-PASEF proteomic analysis of HNSCC tumor and stroma enriched sections from FFPE samples prepared with laser capture microdissection;** Matthew Willetts<sup>1</sup>; Aswini Panigrahi<sup>2</sup>; Diego Assis<sup>1</sup>; Radoslav Goldman<sup>2</sup>; Allison Hunt<sup>3</sup>; Thomas P Conrads<sup>3</sup>; <sup>1</sup>Bruker Scientific, LLC, Billerica, MA; <sup>2</sup>Georgetown University, Washington Dc, DC; <sup>3</sup>Women's Health Integrated Research Center, Annandale, VA
- WP 761 **A Deep Proteome and Protein Complex Analysis of Human Kidney Aging and Diseases;** Thao Nguyen<sup>1</sup>; Niclas Olsson<sup>1</sup>; Leanne J.G. Chan<sup>1</sup>; Wenzhou Li<sup>1</sup>; Phil Seitzer<sup>1</sup>; Aleksandr Gaun<sup>1</sup>; Edward L. Huttlin<sup>1,2</sup>; Daigoro Hirohama<sup>3</sup>; Katalin Susztak<sup>3</sup>; Fiona McAllister<sup>1</sup>; <sup>1</sup>Calico Life Sciences, South San Francisco, CA; <sup>2</sup>Department of Cell Biology, Harvard Medical School, Boston, MA; <sup>3</sup>Renal, Electrolyte, and Hypertension Division, Department of Medicine, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA
- WP 762 **Unlocking the proteomic potential of FFPE tissues with BeatBox and iST: A xylene-free, high-throughput workflow for in-depth proteome analysis;** Brianne Nunez<sup>1</sup>; Katharina Limm<sup>2</sup>; Silvia Wuertenberger<sup>2</sup>; Katrin Hartinger<sup>2</sup>; Jonathan R Krieger<sup>3</sup>; Nils A. Kulak<sup>2</sup>; <sup>1</sup>PreOmics, Billerica, MA; <sup>2</sup>PreOmics, Planegg/Martinsried, Germany; <sup>3</sup>Bruker Canada Ltd, Milton, ON
- WP 763 **High-throughput, streamlined processing workflow of formalin-fixed paraffin-embedded (FFPE) tissue yielding up to 10,000 proteins per sample;** Moe Haines<sup>1</sup>; John Thorup<sup>1</sup>; Simone Gohsman<sup>1</sup>; Lilian Heil<sup>2</sup>; Lia Abarzua<sup>3</sup>; Sameer Vasantgadkar<sup>3</sup>; Chelsea Newton<sup>4</sup>; Dan Rohrer<sup>4</sup>; Galen Hostetter<sup>4</sup>; D. R. Mani<sup>1</sup>; Michael A. Gillette<sup>1</sup>; Steven A. Carr<sup>1</sup>; Shankha Satpathy<sup>1</sup>; <sup>1</sup>Broad Institute of MIT and Harvard, Cambridge, MA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Covaris, LLC, Woburn, MA; <sup>4</sup>Van Andel Research Institute, Grand Rapids, MI
- WP 764 **Location! Location! Location! Deep topographic proteomics from tissue culture to a human brain tumor;** Simon Davis<sup>1</sup>; Yixin Shi<sup>2</sup>; Olaf Ansorge<sup>2</sup>; Philip Charles<sup>2</sup>; Stephen Taylor<sup>2</sup>; Roman Fischer<sup>2</sup>; <sup>1</sup>University of Oxford, Oxford, United Kingdom; <sup>2</sup>University of Oxford, UK, Oxford, United Kingdom
- WP 765 **A Protocol Fast-Tracking Sample Preparation for Proteomics of Formalin Fixed Paraffin Embedded Tumor Tissues;** Lancia N.F. Darville-Bowleg<sup>1</sup>; John H. Lockhart<sup>1</sup>; Sudhir Putty Reddy<sup>1</sup>; Bin Fang<sup>1</sup>; Victoria Izumi<sup>1</sup>; Theresa A. Boyle<sup>1</sup>; Eric B. Haura<sup>1</sup>; Elsa R. Flores<sup>1</sup>; John M. Koomen<sup>1</sup>; <sup>1</sup>Moffitt Cancer Center, Tampa, FL
- WP 766 **Comprehensive Analysis of FFPE Sections through Mass Spectrometry-Based Proteomics in a Fully Automated Workflow;** Paola Pisano<sup>1</sup>; Jonathan Samuel Achter<sup>2</sup>; Emma Maria Åhrman<sup>1</sup>; Katarzyna Izabela Wozniak<sup>1</sup>; Michele Puglia<sup>1</sup>; Irina Pozdnyakova<sup>1</sup>; Cristina Gil Gonzalez<sup>1</sup>; Alicia Lundby<sup>2</sup>; Michael Wierer<sup>1</sup>; <sup>1</sup>Proteomics Research Infrastructure, Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark; <sup>2</sup>Department of Biomedical Sciences, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark
- WP 767 **Quantitative analysis and kinetics of Aβ and Tau proteoforms in living human brains;** Reid A Coyle<sup>1</sup>; Soumya Mukherjee<sup>2</sup>; Aram Aslanyan<sup>3</sup>; Yingxin He<sup>2</sup>; Chihiro Sato<sup>2</sup>; Nupur Ghoshal<sup>2</sup>; Junyue Ge<sup>4</sup>; Srinivas Koutarapu<sup>4</sup>; Katherine Schwetye<sup>2</sup>; Kaleigh Roberts<sup>2</sup>; Don Elbert<sup>5</sup>; Jorg Hanrieder<sup>3, 4</sup>; Randall J Bateman<sup>2</sup>; Ross W Paterson<sup>3</sup>; <sup>1</sup>Washington University St. Louis, St. Louis, MO; <sup>2</sup>Washington University School of Medicine, St. Louis, MO; <sup>3</sup>University College London, London, United Kingdom; <sup>4</sup>University of Gothenburg, Gothenburg, Sweden; <sup>5</sup>University of Washington, Seattle, WA
- WP 768 **The proteome of human and cynomolgus liver;** Yasaman Jami-Alahmadi<sup>1</sup>; Hendrik Neubert<sup>1</sup>; Katherine Wright<sup>1</sup>; Joel Federspiel<sup>1</sup>; Robert Joseph Seward<sup>1</sup>; Pierre M Jean Beltran<sup>2</sup>; <sup>1</sup>Pfizer Inc., Andover, MA; <sup>2</sup>Pfizer, Inc, Cambridge, MA
- WP 769 **Uncovering the Link Between Chronic Inflammation and Alzheimer's Disease Using Label-Free Mass Spectrometry;** Yijun Chen<sup>1</sup>; Xuemei Zeng<sup>2</sup>; Xinfeng Guo<sup>1</sup>; Xiaohai Wang<sup>1</sup>; Thomas K. Karikari<sup>1</sup>; <sup>1</sup>University of Pittsburgh, Pittsburgh, PA; <sup>2</sup>Department of Psychiatry, School of Medicine, University of Pittsburgh, Pittsburgh, Pennsylvania
- WP 770 **Deep-coverage Proteomics using a Photocleavable Surfactant Reveals Extracellular Matrix Alterations in Ischemic Cardiomyopathy;** Kevin M Buck<sup>1</sup>; Holden T Rogers<sup>2</sup>; Morgan W. Mann<sup>3</sup>; Timothy Aballo<sup>2</sup>; Zhan Gao<sup>2</sup>; Emily A Chapman<sup>2</sup>; Scott J Price<sup>2</sup>; Ying Ge<sup>2</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI; <sup>2</sup>UW-MADISON, Madison, WI; <sup>3</sup>Stanford University - Pathology, Stanford, CA
- WP 771 **Single tissue proteomics in Caenorhabditis elegans reveals proteins resident in intestinal lysosome-related**

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- organelles.; Ting-Yu Wang<sup>1</sup>; Chieh-Hsiang Tan<sup>1</sup>; Heenam Park<sup>1</sup>; Brett Lomenick<sup>1</sup>; Tsui-Fen Chou<sup>1</sup>; Paul W. Sternberg<sup>1</sup>; <sup>1</sup>California Institute of Technology, Pasadena, CA
- WP 772 **Leveraging the Covaris AFA-sonication to develop a high-throughput assay for deep proteome coverage of fresh frozen tissue sections;** Saeed Sevedmohammad; Cedars Sinai Medical Institute, Los Angeles, CA
- SINGLE CELL MS III**  
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- WP 773 **Single-Cell Metabolic Fingerprints Discover a Cluster of Circulating Tumor Cells with Distinct Metastatic Potential;** Yun Chen<sup>1</sup>; Feifei Xu<sup>1</sup>; Wenjun Zhang<sup>1</sup>; <sup>1</sup>Nanjing Medical University, Nanjing, China
- WP 774 **Elemental Analysis in yeast cells and selenium enriched yeast cells by ICP-MS with Automated Micro-Flow Sample Introduction;** Yan Cheung<sup>1</sup>; Emmett Soffey<sup>1</sup>; <sup>1</sup>Agilent Technologies, Wood Dale, IL
- WP 775 **Expanding the limits of targeted quantitation for low input proteomics using a novel high-speed hybrid nominal mass instrument;** Chris Hsu<sup>1</sup>; Lilian R Heil<sup>2</sup>; Philip M. Remes<sup>2</sup>; Cristina Jacob<sup>2</sup>; Deanna L. Plubell<sup>1</sup>; Bo Wen<sup>3</sup>; Ritin Sharma<sup>4</sup>; Joshua Cantlon<sup>5</sup>; Jesse D. Canterbury<sup>2</sup>; Ping Yip<sup>2</sup>; William Barshop<sup>2</sup>; Vane Shen<sup>2</sup>; Dani Asapu<sup>2</sup>; Claudia Martins<sup>2</sup>; Scott Peterman<sup>2</sup>; Patrick Pirrotte<sup>4</sup>; Mariya T. Sweetwyne<sup>1</sup>; Christine C. Wu<sup>1</sup>; Michael J. MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>University of Washington, Seattle, WA; <sup>4</sup>The Translational Genomics Research Institute, Phoenix, AZ; <sup>5</sup>Scienion, Phoenix, AZ
- WP 776 **Streamlined High-Throughput Single-Cell Proteomics: Tip-Based Sample Preparation for Enhanced Sensitivity and PTM Identification;** Jongmin Woo<sup>1</sup>; Hongyi Liu<sup>1</sup>; Zhenyu Sun<sup>1</sup>; Yuefan Wang<sup>1</sup>; Lijun Chen<sup>1</sup>; Liyuan Jiao<sup>1</sup>; Kay Li<sup>1</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- WP 777 **Investigating cellular diversity through label-free single-cell proteomics;** Qi Wu<sup>1</sup>; Lei Cheng<sup>1</sup>; Robert A. Fenton<sup>1</sup>; <sup>1</sup>Aarhus University, Aarhus, Denmark
- WP 778 **Exploration of Single Cell Lipidomics with a Novel Multi-reflecting Q-ToF Platform;** Scarlet A Ferrinho<sup>1, 2</sup>; Nyasha Munjoma<sup>2</sup>; Richard Lock<sup>2</sup>; David Heywood<sup>2</sup>; Robert S Plumb<sup>2</sup>; Preeti Mourya<sup>1</sup>; Shazneil Briones<sup>1</sup>; Lee A Gethings<sup>2</sup>; Olivier Cexus<sup>1</sup>; Paul A Townsend<sup>1</sup>; <sup>1</sup>University of Surrey, Guildford, United Kingdom; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom
- WP 779 **Single-cell multi-omics analysis of in vitro post-ovulatory aged oocytes revealed aging-dependent protein degradation;** Xuejiang Guo<sup>1</sup>; Yueshuai Guo<sup>1</sup>; Mengmeng Gao<sup>1</sup>; Xiaofei Liu<sup>1</sup>; Haotian Zhang<sup>1</sup>; Chenghao Situ<sup>1</sup>; Yan Li<sup>1</sup>; <sup>1</sup>State Key Laboratory of Reproductive Medicine and Offspring Health, Nanjing Medical University, Nanjing, China
- WP 780 **Elevating Single-Cell Proteomics: Maximizing Sensitivity and Throughput with Advanced Chromatographic Separation and MS Data Acquisition Strategies;** Runsheng Zheng<sup>1</sup>; Manuel Matzinger<sup>2</sup>; Rupert Mayer<sup>2</sup>; Tabiwang N Arrey<sup>3</sup>; Alec Valenta<sup>1</sup>; Xufei Sun<sup>4</sup>; Christopher Pynn<sup>1</sup>; Ece Aydin<sup>1</sup>; Wim Decrop<sup>1</sup>; Dominic Hoch<sup>5</sup>; Martin Samonig<sup>1</sup>; Karl Mechtler<sup>2, 6, 7</sup>; <sup>1</sup>Thermo Fisher Scientific, Germering, Germany; <sup>2</sup>Institute of Molecular Pathology, Campus-Vienna-Biocenter 1, Vienna, Austria; <sup>3</sup>Thermo Fisher Scientific GmbH, Bremen, Germany; <sup>4</sup>Thermo Fisher Scientific, Sunnyvale, CA; <sup>5</sup>Thermo Fisher Scientific, Reinach, Switzerland; <sup>6</sup>Institute of Molecular Biotechnology of the Austrian Academy of Sciences, Vienna, Austria; <sup>7</sup>Gregor Mendel Institute of Molecular Plant Biology of the Austrian Academy of Sciences, Vienna, Austria
- WP 781 **Deep single-cell proteomics of human induced pluripotent stem cells differentiation provides a time-lapse of cell-type specific protein markers;** Pierre Sabatier<sup>1, 2</sup>; Zilu Ye<sup>1, 3</sup>; Maico Lechner<sup>1</sup>; Sergey Rodin<sup>2</sup>; Karl-Henrik Grinnemo<sup>2</sup>; Jesper Velgaard Olsen<sup>1</sup>; <sup>1</sup>Novo Nordisk Foundation Center for Protein Research, Proteomics Program, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; <sup>2</sup>Department of Surgical Sciences, Uppsala University, Uppsala, Sweden; <sup>3</sup>State Key Laboratory of Common Mechanism Research for Major Diseases, Suzhou Institute of Systems Medicine, Suzhou, China
- WP 782 **Single cell Deep Visual Proteomics allows precise spatial mapping of proteomic changes in human liver tissue;** Caroline Weiss<sup>1</sup>; Lauryn Brown<sup>2</sup>; Paolo Pellizoni<sup>3</sup>; Lucas Miranda<sup>3</sup>; Marvin Thielert<sup>1</sup>; Jonathan Hernandez<sup>4</sup>; Karsten Borgwardt<sup>3</sup>; Natalie Porat-Shilom<sup>2</sup>; Florian Rosenberger<sup>1</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Martinsried, Germany; <sup>2</sup>Thoracic and GI Malignancies Branch, National Cancer Institute, National Institutes of Health, Bethesda, MD; <sup>3</sup>Machine Learning and Systems Biology, Max Planck Institute of Biochemistry, Martinsried, Germany; <sup>4</sup>Surgical Oncology Program, National Cancer Institute, National Institutes of Health, Bethesda, MD
- WP 783 **Phospholipid analysis of single-cells by live single-cell mass spectrometry;** Hajime Mizuno<sup>1</sup>; Aogu Furusho<sup>2</sup>; Jo Sakata<sup>2</sup>; Takuma Yanagisawa<sup>1, 2</sup>; Eiji Sugiyama<sup>2</sup>; Susumu Y. Imanishi<sup>1</sup>; Kenichiro Todoroki<sup>2</sup>; Iwao Sakane<sup>3</sup>; <sup>1</sup>Meijo University, Nagoya, Japan; <sup>2</sup>University of Shizuoka, Shizuoka, Japan; <sup>3</sup>ITO EN Ltd., Makinohara, Japan
- WP 784 **Single-cell proteomics by mass spectrometry of pre-implantation mouse embryos uncover distinct asymmetry of certain proteins among early blastomeres;** Yuan Yuan<sup>1</sup>; Mo Hu<sup>2</sup>; Yinghui Zheng<sup>1</sup>; Xiaoliang Sunney Xie<sup>1</sup>; <sup>1</sup>Peking University, Beijing, China; <sup>2</sup>Changping Laboratory, Beijing, China
- WP 785 **Challenging the Astral mass analyzer - going beyond 5200 proteins per single-cell at unseen quantitative accuracy studying cell cycle biology;** Manuel Matzinger<sup>1</sup>; Julia A Bubis<sup>1</sup>; Tabiwang N Arrey<sup>2</sup>; Eugen Damoc<sup>2</sup>; Bernard Delanghe<sup>2</sup>; Karl Mechtler<sup>1</sup>; <sup>1</sup>Protein Chemistry Group, IMP, Vienna, Austria; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany
- WP 786 **High throughput single-cell mass spectrometry enabling structural elucidation and relative quantitation of phospholipid C=C isomers;** Chenxi Cao<sup>1</sup>; Simin Cheng<sup>2</sup>; Yao Qian<sup>1</sup>; Zheng Ouyang<sup>1</sup>; Xiaoxiao Ma<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>National Institute of Metrology, Beijing, China
- WP 787 **Label-free DIA-based workflow for single-cell proteomic analysis on an Orbitrap Ascend Tribrid mass spectrometer;** Fernanda Salvato<sup>1</sup>; Julia Kraegenbring<sup>2</sup>; Bernard Delanghe<sup>2</sup>; David Hartmayr<sup>3</sup>; Anjali Seth<sup>3</sup>; Amirmansoor Hakimi<sup>1</sup>; Tonya Pekar Hart<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Cellenion, Lyon, France
- WP 788 **High-throughput Lipidomic Profiling of Individual Mammalian Mitochondria using Image-guided MALDI-2 Mass Spectrometry;** Seth W Croslow<sup>1, 2</sup>; Timothy J Trinklein<sup>1</sup>; Stanislav Rubakhin<sup>1, 2</sup>; Jonathan Sweedler<sup>1, 2</sup>; <sup>1</sup>Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Champaign, IL; <sup>2</sup>Department of Chemistry, University of Illinois Urbana-Champaign, Champaign, IL
- WP 789 **Going Viral: Sex Heterogeneity of Human Astrocytes' Infection Response through Single-Cell Proteomics;** Shuxin Chi<sup>1</sup>; Arpa Ebrahimi<sup>2</sup>; Jason Rogalski<sup>1</sup>; Claudia Maier<sup>2</sup>; Leonard J Foster<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, BC; <sup>2</sup>Oregon State University, Corvallis, OR
- WP 790 **Gradient Elution Nanoflow Liquid Chromatography without a Binary Pump: Smoothed Step Gradients Enable Inexpensive, Sensitive and Reproducible Single-Cell Proteomics;** Kei Webber<sup>1</sup>; Siqi Huang<sup>1</sup>; Lavender Lin<sup>1</sup>; Tyler Hunter<sup>1</sup>; Josh Andersen<sup>2</sup>; Ryan T. Kelly<sup>1, 3</sup>; <sup>1</sup>Brigham Young University, Provo, UT; <sup>2</sup>University of Utah, Salt Lake City, UT; <sup>3</sup>MicroOmics Technologies, Spanish Fork, UT
- WP 791 **High-Throughput Profiling of Lipids and Targeted Proteins Using Microscopy-Guided Single Cell Mass**

## WEDNESDAY POSTERS

- Spectrometry**; Marisa Asadian<sup>1</sup>; Timothy J Trinklein<sup>1</sup>; Stanislav Rubakhin<sup>1</sup>; Mark J. Lim<sup>2</sup>; Gargey Yagnik<sup>2</sup>; Orly Lazarov<sup>3</sup>; Fan Lam<sup>1</sup>; Kenneth J. Rothschild<sup>2, 4</sup>; Jonathan V. Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign, Champaign, Illinois; <sup>2</sup>AmberGen Inc., Billerica, MA; <sup>3</sup>University of Illinois at Chicago, Chicago, IL; <sup>4</sup>Boston University, Department of Physics and Photonics Center, Boston, MA
- WP 792 **Single-cell and low-input proteomics depicted an in-depth landscape for mouse maternal-to-zygotic transition**; Chen Li; Center for Single-Cell Omics, School of Medicine, Shanghai Jiao Tong University, Shanghai, China
- WP 793 **Single Cell Metabolomics and Proteomics Studies of CRISPR/Cas9 Gene Editing Results**; Tra D Nguyen<sup>1</sup>; Lindsay Martin<sup>1</sup>; Zongkai Peng<sup>1</sup>; Eniola A Adewunmi<sup>2</sup>; Neeraj K Chauhan<sup>2</sup>; Shakya Sankalpani Gunasena Wijie Munige<sup>1</sup>; Deepti Bhusal<sup>1</sup>; Rakhi Rajan<sup>1</sup>; Martin-Paul Agbaga<sup>2</sup>; Zhibo Yang<sup>1</sup>; <sup>1</sup>University of Oklahoma, Norman, OK; <sup>2</sup>The University of Oklahoma Health Sciences Center, Oklahoma City, Oklahoma
- WP 794 **In-depth Proteome Profiling of <1000 bacterial cells**; Andikan Jones Nwosu<sup>1</sup>; Madi Johnston<sup>1</sup>; Cecile Thion<sup>2</sup>; Siqi Huang<sup>3</sup>; Xiaofeng Xie<sup>3</sup>; Ryan T. Kelly<sup>3</sup>; <sup>1</sup>Brigham Young University, Provo, UT; <sup>2</sup>Cellenion, Lyon, France; <sup>3</sup>Brigham Young University, Provo
- SYNTHETIC POLYMERS**  
795-808
- WP 795 **Analysis of aminated polybutadiene via matrix-assisted laser desorption/ionization - time-of-flight mass spectrometry**; Brennan Curole<sup>1</sup>; Sabrina Scott<sup>2</sup>; Laurel L Schafer<sup>2</sup>; Scott Michael Grayson<sup>1</sup>; <sup>1</sup>Tulane University, New Orleans, LA; <sup>2</sup>University of British Columbia, Vancouver, BC
- WP 796 **Coupling Multi-Stage Fragmentation with Ion Mobility-Mass Spectrometry for Serial Sequencing of Blocks in Digital Polymers**; Isaure Sergent<sup>1</sup>; Thibault Schutz<sup>2, 3</sup>; Laurence Oswald<sup>3</sup>; Georgette Obeid<sup>2</sup>; Jean-François Lutz<sup>2, 3</sup>; Laurence Charles<sup>1</sup>; <sup>1</sup>Aix Marseille Université, CNRS, UMR 7273, Institut de Chimie Radicalaire (ICR), Marseille, France; <sup>2</sup>Université de Strasbourg, CNRS, Institut de Science et d'Ingénierie Supramoléculaires (ISIS), Strasbourg, France; <sup>3</sup>Université de Strasbourg, CNRS, Institut Charles Sadron UPR22, Strasbourg, France
- WP 797 **Online Bipolar Dual Spray for the Charge State Reduction and Characterization of Complex Synthetic Polymers**; John Stutzman<sup>1</sup>; Paul D. Hutchins<sup>1</sup>; Ryan M. Bain<sup>1</sup>; <sup>1</sup>Dow Inc, Midland, MI
- WP 798 **Chemical fingerprinting of synthetic polymers using temperature-programmed direct mass spectrometric analysis**; Ville Nissinen<sup>1</sup>; Krista Gronlund<sup>1</sup>; Mika Suvanto<sup>1</sup>; Jarkko J. Saarinen<sup>1</sup>; Janne Janis<sup>1</sup>; <sup>1</sup>University of Eastern Finland, Joensuu, Finland
- WP 799 **Identifying Polymers' DART-HRMS Ions for Food Contact Article Screening**; Victoria M Anderson<sup>1</sup>; Jānis Ruško<sup>2</sup>; Ingus Pērkonis<sup>2</sup>; Kristen L. Reese<sup>3</sup>; Luke K. Ackerman<sup>3</sup>; <sup>1</sup>Joint Institute for Food Safety and Applied Nutrition (JIFSAN), University of Maryland, College Park, MD; <sup>2</sup>BIOR Institute of Food Safety, Animal Health and Environment "BIOR", Laboratory of Chemistry, Leļupes street 3, Riga, Latvia; <sup>3</sup>U.S. Food and Drug Administration, Center for Food Safety and Applied Nutrition, 5001 Campus Drive, College Park, MD
- WP 800 **Rapid Characterization of Crosslinked Networks by Thermal Desorption/Pyrolysis Interfaced to Direct Analysis in Real Time Mass Spectrometry (TDPy-DART-MS)**; Calum Bochenek<sup>1</sup>; Tyler C Arntz<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>The University of Akron, Akron, OH
- WP 801 **Identification of Linear-Dendritic Copolymer Structures via MALDI-TOF MS**; Ashley Miles<sup>1</sup>; Allycea Huskey<sup>1</sup>; Anna Nuzzo<sup>1</sup>; Scott M Grayson<sup>1</sup>; <sup>1</sup>Tulane University, New Orleans, LA
- WP 802 **Synthesis of Linear and Cyclic Poly(hydroxypivalic acid)**; Amman Nadeem<sup>1</sup>; Lavinia Moon Palmer<sup>1</sup>; Scott Michael Grayson<sup>1</sup>; <sup>1</sup>Tulane University, New Orleans, LA
- WP 803 **The use of soft ionization in the creation of a searchable pyrolysis GC/MS mass spectral library**; Edward Erisman<sup>1</sup>; Yamil Simón-Manso<sup>1</sup>; William E Wallace<sup>1</sup>; Stephen E Stein<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD
- WP 804 **Graphical Data Analysis and Sample Comparison of Complex Mesophase Pitches**; Mark A Arnould<sup>1</sup>; Aparna Annamraju<sup>2</sup>; Ercan Cakmak<sup>2</sup>; Frederic Vautard<sup>2</sup>; <sup>1</sup>Bruker Scientific, LLC, Billerica, MA; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN
- WP 805 **MALDI-TOF MS Analysis of Mechanopolymers and Vitrimers**; Kushal Modi<sup>1</sup>; Mark A Arnould<sup>1</sup>; Chrys Wesdemiotis<sup>2</sup>; Calum Bochenek<sup>2</sup>; Tyler Arntz<sup>2</sup>; <sup>1</sup>Bruker Scientific, LLC, Billerica, MA; <sup>2</sup>The University of Akron, Akron, OH
- WP 806 **Investigating the cyclization of linear ethylene brassylate through MALDI-MS**; Mahi Ahmad<sup>1</sup>; Scott Michael Grayson<sup>1</sup>; <sup>1</sup>Tulane University, New Orleans, LA
- WP 807 **Examination of Self-Healing Thermosets Through Thermal Degradation: Pyrolysis Direct Analysis in Real Time (TDPy-DART-MS) and MALDI Structural Profiling**; Tyler C Arntz<sup>1</sup>; Calum Bochenek<sup>1</sup>; Bryan Katzenmeyer<sup>2</sup>; Robert B Cody<sup>2</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>The University of Akron, Akron, OH; <sup>2</sup>JEOL USA, Inc., Peabody, MA
- WP 808 **Deciphering the secrets of environmental polyethylene terephthalates microplastics (PET) by chemical depolymerization and advanced mass spectrometry**; Bayan ALMASRI<sup>1, 2</sup>; Youssef BAKKOUR<sup>2, 3</sup>; Christian ROLANDO<sup>1, 4</sup>; <sup>1</sup>Miniaturization for Synthesis, Analysis & Proteomics (MSAP), USR 3290, CNRS, University of Lille, Faculty of Sciences & Technologies, Villeneuve d'Ascq, France; <sup>2</sup>Laboratory of Applied Chemistry (LAC), Lebanese University, Faculty of Sciences, Tripoli, Lebanon; <sup>3</sup>King Khalid University, Abha, Saudi Arabia; <sup>4</sup>Shrieking Sixties, 1-3 Allée Lavoisier, Villeneuve d'Ascq, France
- TOXICOLOGY**  
809-821
- WP 809 **A Coated Blade Spray Mass Spectrometry Workflow for Rapid Toxicology General Unknown Screening**; David Borts<sup>1</sup>; Laura Burns<sup>1</sup>; Dwayne Schrunck<sup>1</sup>; Shane Stevens<sup>2</sup>; Ryan Micklitsch<sup>2</sup>; <sup>1</sup>Iowa State University, Ames, IA; <sup>2</sup>Restek Corporation, Bellefonte, PA
- WP 810 **A Triple Quadrupole GC/MS MRM Database for Forensic and Toxicological Workflows**; Celine Gys<sup>1</sup>; Anna Klimowska<sup>1, 2</sup>; Adrian Covaci<sup>1</sup>; Remko Van Loon<sup>3</sup>; Joel Ferrer<sup>4</sup>; Anastasia Andrianova<sup>5</sup>; <sup>1</sup>Toxicological Center, University of Antwerp, Antwerp, Belgium; <sup>2</sup>Department of Toxicology, Medical University of Gdansk, Gdansk, Poland; <sup>3</sup>Agilent Technologies, Middelburg, Netherlands; <sup>4</sup>Agilent Technologies, Santa Clara, CA; <sup>5</sup>Agilent Technologies, Wilmington, DE
- WP 811 **Rapid Assessment of Toxicants in Emergency Care with Ambient Ionization Mass Spectrometry**; Yi-Wen Hsu<sup>1</sup>; Hung Su<sup>2</sup>; Chi-Wei Lee<sup>1</sup>; Jentaie Shiea<sup>2</sup>; <sup>1</sup>Institute of Medical Science and Technology, National Sun Yat-sen University, Kaohsiung, Taiwan; <sup>2</sup>Department of Chemistry, National Sun Yat-sen University, Kaohsiung, Taiwan
- WP 812 **Exploring the Toxicity Mechanism of CsPbBr<sub>2</sub>I Perovskite Quantum Dots by Mass Spectrometry-based Metabolomics**; Cristina Gutierrez Lopez<sup>1</sup>; Gabriel A. Peñalver<sup>1</sup>; Andres Machuca<sup>1</sup>; Estefania Garcia-Calvo<sup>1</sup>; Jose L. Luque-Garcia<sup>1</sup>; <sup>1</sup>Complutense University of Madrid, Madrid, Spain
- WP 813 **Species-Specific Profiles of Per- and Polyfluoroalkyl Substances in Small Coastal Sharks Along the South Atlantic Bight of the United States**; Qaim Mehdi<sup>1</sup>; Emily K Griffin<sup>1</sup>; Juliette Esplugas<sup>1</sup>; Ashley S Galloway<sup>2</sup>; Bryan S Frazier<sup>3</sup>; Alina S Timshina<sup>1</sup>; R Dean Grubbs<sup>4</sup>; Keyla Correia<sup>1</sup>; Camden G Camacho<sup>1</sup>; Jim Gelsleichter<sup>5</sup>; John Bowden<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>South Carolina Department of Natural Resources Marine Resources Division, Charleston, South Carolina; <sup>3</sup>South Carolina Department of Natural Resources Marine Resources Division, Charleston, USA; <sup>4</sup>Florida State University, St.

## WEDNESDAY POSTERS

- Teresa, Florida; <sup>5</sup>University of North Florida, Jacksonville, Florida
- WP 814 **Optimized Sample Preparation for Low Level Determination of the Alcohol Marker EtG from Hair Using UPLC-MS/MS Analysis;** Lee Williams<sup>1</sup>; Zainab Khan<sup>1</sup>; Lucy Lund<sup>1</sup>; Adam Senior<sup>1</sup>; Helen Lodder<sup>1</sup>; Russell Parry<sup>1</sup>; Geoff Davies<sup>1</sup>; Alan Edgington<sup>1</sup>; Claire Desbrow<sup>1</sup>; Dan Menasco<sup>1</sup>; Esraa AboJasser<sup>1</sup>; <sup>1</sup>Biotage GB Limited, Cardiff, United Kingdom
- WP 815 **Evaluating the proteome profiles in juvenile Coho gill and liver tissues exposed to the toxic tire-associated contaminant 6PPD-quinone;** Jason Rogalski<sup>1</sup>; Bonnie P Lo<sup>2</sup>; Xiaojing Yuan<sup>1</sup>; Lok Tin Hui<sup>1</sup>; Vicki L Marlatt<sup>2</sup>; Tanya M Brown<sup>2</sup>; <sup>1</sup>University of British Columbia, Vancouver, BC; <sup>2</sup>Simon Fraser University, Burnaby, BC
- WP 816 **Untargeted LC-MS/MS Analysis of Drug Metabolites in Human Hepatocyte Suspensions for Comparison to Rat Liver S9 Fractions;** Tyler S. Larson<sup>1</sup>; Krishna Ravindra<sup>2</sup>; Barbara A. Wetmore<sup>3</sup>; Denise K. MacMillan<sup>3</sup>; <sup>1</sup>Oak Ridge Institute for Science and Education, Oak Ridge, TN; <sup>2</sup>Oak Ridge Associated Universities, Oak Ridge, Tennessee; <sup>3</sup>US Environmental Protection Agency, Research Triangle Park, NC
- WP 817 **Characterization of a Humanized Mouse Model of Organophosphate Poisoning and Detection of Countermeasures via MALDI-MSI;** Caitlin Tressler<sup>1</sup>; Benjamin Wadsworth<sup>2</sup>; Samantha Carriero<sup>2</sup>; Natalie Dillman<sup>1</sup>; Rachel Crawford<sup>1</sup>; C. Linn Cadieux<sup>2</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>US Army Medical Research Institute for Chemical Defense, Aberdeen Proving Ground, MD
- WP 818 **LC-MS/MS Analysis to Evaluate Hepatotoxicity of Therapeutic Molecules in Cell Media of Complex Liver In Vitro Models;** France Landry<sup>1</sup>; Yongliang (Kevin) Zhang<sup>1</sup>; Vasanthi Bhaskaran<sup>1</sup>; Alexa Murray<sup>2</sup>; Rhiannon Hardwick<sup>2</sup>; Patrick Devine<sup>3</sup>; Petia Shipkova<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb, Lawrenceville, NJ; <sup>2</sup>Bristol Myers Squibb, San Diego, CA; <sup>3</sup>Bristol Myers Squibb, Cambridge, MA
- WP 819 **Application of High Resolution LC/MS Analysis to In Vitro Comparative Metabolism (IVCM) Samples for the Fungicide Crop Protection Chemical Oxathiapiprolin;** Michael P Mawn<sup>1</sup>; Lingshuang Cai<sup>1</sup>; Vitaly Palamarchouk<sup>1</sup>; Leonid Khyliuk<sup>1</sup>; Jen Goodell<sup>1</sup>; Matthew W Himmelstein<sup>1</sup>; <sup>1</sup>Corteva Agriscience, Newark, DE
- WP 820 **Rapid high-resolution screening for drugs of abuse with library searching on a novel acoustic ejection HRMS with triple quadrupole confirmation;** Aaron Stella<sup>1</sup>; Jacob McCabe<sup>1</sup>; Anuja Bhalkikar<sup>2</sup>; <sup>1</sup>SCIEX, USA, Framingham, MA; <sup>2</sup>Sciex, Framingham, MA
- WP 821 **Direct determination of 12 drugs of abuse in saliva using new LDTD Ion Source at 8 seconds per sample;** Jean Lacoursière<sup>1</sup>; Jonathan Rochon<sup>1</sup>; Mégane Moreau<sup>1</sup>; Sarah Demers<sup>1</sup>; Serge Auger<sup>1</sup>; Pierre Picard<sup>1</sup>; <sup>1</sup>Phytronix Technologies, Quebec, QC

## THURSDAY POSTERS

### THURSDAY POSTERS

Set up all Thursday posters  
6:30 - 9:00 am

**Odd-numbered posters present**  
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

**Even-numbered posters present**  
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Thursday posters  
**2:30 - 3:00 pm**

Antibodies & Antibody Drug Conjugates II.....	001-032
Art, Archaeology & Paleontology.....	033-041
Artificial Intelligence in MS Instrumentation and Applications II.....	042-069
Biomarkers: Discovery II.....	070-099
Biomarkers: Quantitative Analysis III.....	100-126
Cancer Research II.....	127-160
Clinical Analysis II.....	161-187
Covalent Labeling and Chemical Crosslinking II.....	188-212
Drug Discovery: Qualitative and Quantitative Analysis II.....	213-237
Epigenetic Modifications.....	238-244
Food Safety: General.....	245-273
Forensics.....	274-303
Fundamentals: Ion Spectroscopy.....	304-308
Fundamentals: Ionic Clusters, Nanomaterials, and Catalysis.....	309-311
Fundamentals: Ionization.....	312-325
GC/MS: Instrumentation and Applications.....	326-364
Glycoproteins II.....	365-393
High Mass Accuracy/High Performance MS: Applications.....	394-412
Imaging MS: Computational Methods, Software, and Analysis.....	413-429
Imaging MS: Disease Markers.....	430-442
Imaging MS: Method Development II.....	443-476
Informatics: General, SRM, and DIA.....	477-484
Informatics: Multiomics Integration.....	485-502
Instrumentation: New Concepts.....	503-519
Instrumentation: New Developments in Ionization and Sampling.....	520-538
Ion Mobility: Fundamentals.....	539-544
Ion Mobility: Structure.....	545-565
LC/MS: General.....	566-594
Lipids: Targeted and Quantitative Analysis.....	595-627
MALDI: Applications.....	628-638
MALDI: Innovation in Instrumentation and Sample Preparation.....	639-644
Metabolomics: Targeted and Quantitative Analysis II.....	645-666
Natural Products.....	667-694
Proteins: PTMs II.....	695-715
Proteomics: Clinical Applications II.....	716-737
Proteomics: Intact Proteins and Top Down Analysis II.....	738-767
Proteomics: Quantitative II.....	768-799
Systems Biology.....	800-815

### ANTIBODIES & ANTIBODY DRUG CONJUGATES II 001-032

- ThP 001 **Charge variant identification and localization of post-translational modifications with integrated iCIEF-UV/MS;** Scott Mack<sup>1</sup>; Jingwen Ding<sup>1</sup>; Zoe Zhang<sup>2</sup>; Maggie Ostrowski<sup>1</sup>; <sup>1</sup>SCIEX, Fremont, CA; <sup>2</sup>SCIEX, Redwood City, CA
- ThP 002 **Nanoparticle-based enrichment provides deeper insight into host cell proteins in biological drug products;** Samira Vautrin<sup>1</sup>; Emmanuel Nony<sup>2</sup>; <sup>1</sup>Evotec, München, Germany; <sup>2</sup>Servier R&D Institute, Gif-sur-Yvette, France
- ThP 003 **Data Independent LC-MS Assays for Identification, Quantification and Monitoring of Host Cell Proteins in Monoclonal Antibodies;** Catalin E Doneanu<sup>1</sup>; Scott Berger<sup>1</sup>; Ying Qing Yu<sup>1</sup>; Sean Wu<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA
- ThP 004 **Determination of drug-to-antibody ratio of antibody-drug conjugate in biological samples using microflow-liquid chromatography/high-resolution mass spectrometry;** Kazuko Inoue<sup>1</sup>; Ayako Kurimoto<sup>2</sup>; Toshiki Mochizuki<sup>1</sup>; Nana Kasamori<sup>1</sup>; Takafumi Komori<sup>1</sup>; <sup>1</sup>Eisai Co.,Ltd., Tsukuba, Japan; <sup>2</sup>Protein Metrics, LLC, Cupertino, CA
- ThP 005 **Disulfide Bond Mapping of Cysteine-Engineered Biotherapeutics;** Scott Ugrin<sup>1</sup>; John E Harlan<sup>1</sup>; <sup>1</sup>AbbVie Inc., North Chicago, IL
- ThP 006 **Charge variant analysis of antibody-drug conjugates using an iCIEF-UV/MS approach;** Rashmi Madda<sup>1</sup>; Jingwen Ding<sup>2</sup>; Haichuan Liu<sup>1</sup>; Scott Mack<sup>2</sup>; Maggie Ostrowski<sup>2</sup>; Steven Calciano<sup>2</sup>; Zoe Zhang<sup>1</sup>; <sup>1</sup>SCIEX, Redwood City, CA; <sup>2</sup>SCIEX, Fremont, CA
- ThP 007 **Identification of the Root Cause of Particle Formation in a Therapeutic Monoclonal Antibody by LC-MS-Based Approach;** Amareth Lim<sup>1</sup>; Brandon L. Doyle<sup>1</sup>; William D. Holmes<sup>1</sup>; Andrew G. Werner<sup>1</sup>; Andrew W. Carr<sup>1</sup>; Elisabeth Krug<sup>1</sup>; Suzanne E. Stone<sup>1</sup>; <sup>1</sup>Eli Lilly and Company, Indianapolis, IN
- ThP 008 **Middle-Down MS with Orbitrap-Based Electron Capture Dissociation Reveals Structural Changes of Monoclonal Antibodies After Being Subjected to Forced Degradation Conditions;** XuanYu Chen<sup>1</sup>; Benqian Wei<sup>1</sup>; Joseph Loo<sup>1</sup>; Rachel Loo<sup>1</sup>; <sup>1</sup>University of California Los Angeles, Los Angeles, CA
- ThP 009 **Imaged capillary isoelectric focusing – Mass Spectrometry (iCIEF- MS) online coupling for polatuzumab vedotin charge heterogeneity analysis using native MS;** Xiaoxi Zhang<sup>1</sup>; Tony Chen<sup>2</sup>; Tao Bo<sup>2</sup>; Tiemin Huang<sup>2</sup>; Min Du<sup>3</sup>; <sup>1</sup>ThermoFisher Scientific, Shanghai, China; <sup>2</sup>Advanced Electrophoresis Solutions Ltd, Cambridge, ON; <sup>3</sup>Thermo Fisher Scientific, Lexington, MA
- ThP 010 **Advancements in Sensitivity: Enhancing Analytical Flow LC-MS Method for Host Cell Proteins (HCPs) Identification and Quantitation;** Pingli Wei<sup>1</sup>; Gordon Nicol<sup>1</sup>; Ping Jiang<sup>1</sup>; Jie Ding<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Middleton, WI
- ThP 011 **In-depth Characterization of Stressed Bispecific Antibody and Assessment of Batch Consistency by UHPLC-HRAM MS Based Peptide Mapping;** Sensen Chen<sup>1</sup>; Xiaoxi Zhang<sup>1</sup>; Min Du<sup>2</sup>; <sup>1</sup>ThermoFisher Scientific, Shanghai, China; <sup>2</sup>Thermo Fisher Scientific, Lexington, MA
- ThP 012 **Investigation of IgG subclasses with YTE mutation on Stability Properties of monoclonal antibodies;** Koyuki Takenaka<sup>1,2</sup>; Michael A. Batt<sup>1,2</sup>; Alexandra M. Miller<sup>2</sup>; Qi G. Zhang<sup>1,2</sup>; Jeffrey S. Boyles<sup>2</sup>; Joomi Ahn<sup>1,2</sup>; <sup>1</sup>Lilly Biotechnology Center, San Diego, CA; <sup>2</sup>Eli Lilly and Company, Indianapolis, IN
- ThP 013 **Fluorinated ethylamine-based universal buffer system for native LC-MS analysis of mAbs, ADCs, and other proteins;** Algirdas Velyvis<sup>1</sup>; Siavash Vahidi<sup>1</sup>; <sup>1</sup>University of Guelph, Guelph, ON
- ThP 014 **Improving the Throughput and Accuracy of a Quantitative Method for the PGT 121.414.LS bNAb in Human Serum before Method Validation;** Philip H Lindhorst<sup>1</sup>; Connor Gould<sup>1</sup>; Jill Hochreiter<sup>1</sup>; Qing Ma<sup>1</sup>;

## THURSDAY POSTERS

- Raymond Cha<sup>1</sup>; Robin Difrancesco<sup>1</sup>; Gene D. Morse<sup>1</sup>; Troy D. Wood<sup>1</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY
- ThP 015 **Discovery and Investigation of G0 Glycan Isomers in an Afucosylated Therapeutic Antibody**; Miyang Li<sup>1</sup>; Sean Shen<sup>1</sup>; Simon Letarte<sup>1</sup>; <sup>1</sup>Gilead Sciences Inc, Oceanside, CA
- ThP 016 **CE-MS and the Enhanced Charge Variant Analysis in Site-Specific Antibody-Drug Conjugates**; Leo (Lei) Wang<sup>1</sup>; Paul Shen<sup>2</sup>; Larry (Lei) Wang<sup>1</sup>; Christopher Barton<sup>1</sup>; <sup>1</sup>Takeda, Lexington, MA; <sup>2</sup>Middlebury College, Middlebury, VT
- ThP 017 **Native Mass Spectrometry and Collision Induced Unfolding Reveal Linker-Payload-Dependent Changes in Antibody-Drug Conjugate Higher-Order Structure and Stability**; Devin M. Makey<sup>1</sup>; Marion H. Emmert<sup>2</sup>; Hang Hu<sup>2</sup>; Erik L. Regalado<sup>2</sup>; Rodell C. Barrientos<sup>2</sup>; Brandon T. Ruotolo<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Merck & Co., Inc., Rahway, NJ
- ThP 018 **HPLC/MS Quantitation of Unconjugated Drugs in the Presence of Antibody Drug Conjugates (ADCs)**; Eric W. Ma<sup>1</sup>; William Mylott<sup>1</sup>; <sup>1</sup>PPD, Richmond, VA
- ThP 019 **Disulfide Connectivity in Monoclonal Antibodies: Insights from High-Resolution cIMS-MS Analysis**; Hee-Jin Yoo<sup>1</sup>; Duck-Hyun Kim<sup>1</sup>; Abhik Mojumdar<sup>1</sup>; Kun Cho<sup>1</sup>; <sup>1</sup>Korea Basic Science Institute, Ochang, South Korea
- ThP 020 **Expanding functional antibody characterization to proteoforms: Affinity CE-MS to study antibody proteoform – FcRs interactions**; Christoph Gstöttner<sup>1</sup>; Manfred Wuhrer<sup>1</sup>; Elena Dominguez-Vega<sup>1</sup>; <sup>1</sup>Leiden University Medical Center, Leiden, Netherlands
- ThP 021 **Charge variant microheterogeneity explored via icIEF and offline MS analysis of infliximab biosimilars**; Nora Crushell<sup>1</sup>; Anna Mulligan<sup>1,2</sup>; Sara Carillo<sup>1</sup>; Zarnab Yasmeen<sup>3</sup>; Jean-François Bellec<sup>3</sup>; Jonathan Bones<sup>1,2</sup>; <sup>1</sup>The National Institute for Bioprocessing Research & Training, Dublin, Ireland; <sup>2</sup>School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland; <sup>3</sup>Bio-technie Ltd., Abingdon, United Kingdom
- ThP 022 **Evaluating long-term stability of a monoclonal antibody by using Accelerated Stability Assessment Program modelling and high resolution mass spectrometry**; Geert Van Raemdonck<sup>1</sup>; Kristina Wicht<sup>1</sup>; Kevin Roeleveld<sup>1</sup>; <sup>1</sup>AnaBioTec, Evergem, Belgium
- ThP 023 **Digging into Characterizing the Complexity of Charge Heterogeneity of a Novel Antibody Drug Conjugate by icIEF-UV/MS**; Kristen Niels<sup>1</sup>; Hirsh Nanda<sup>2</sup>; Robert Hepler<sup>2</sup>; Mariam S ElNaggar<sup>3</sup>; Scott Mack<sup>3</sup>; Zoe Zhang<sup>3</sup>; <sup>1</sup>Janssen Biopharmaceuticals, Springhouse, PA; <sup>2</sup>Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania; <sup>3</sup>SCIEX, Fremont, CA
- ThP 024 **LC-MS Based Approaches for Determination of Drug-to-Antibody Ratio of an Antibody Drug Conjugate in Human Plasma**; Lucy WR Gao<sup>1</sup>; Xuefei Zhong<sup>1</sup>; Ying Sheng<sup>1</sup>; Yuan Mao<sup>1</sup>; Tao Xing<sup>1</sup>; Yuetian Yan<sup>1</sup>; Shunhai Wang<sup>1</sup>; Ning Li<sup>1</sup>; Albert Torri<sup>1</sup>; <sup>1</sup>Regeneron Pharmaceuticals, Tarrytown, NY
- ThP 025 **Top-Down CDR Sequencing of Native Intact mAbs Through Deconvolution of HC+LC Mixture Spectra**; Lily E. Miller<sup>1</sup>; Stephanie Sturgeon<sup>2</sup>; Yury V. Vasilev<sup>2</sup>; Rachel Franklin<sup>2</sup>; Blake Hakkila<sup>2</sup>; Timothy Djang<sup>3</sup>; Alex Gavrilenko<sup>3</sup>; Jhenya Gavrilenko<sup>3</sup>; Panos Iatrou<sup>3</sup>; Stelios Gkegkas<sup>3</sup>; Diana Oppenheimer<sup>2</sup>; Derrill Sturgeon<sup>3</sup>; Joseph Meeuswen<sup>2</sup>; Adrian L Guthals<sup>2</sup>; <sup>1</sup>University of Oregon, Eugene, OR; <sup>2</sup>Agilent Technologies, Corvallis, Oregon; <sup>3</sup>Devicepros, Boston, USA, MA
- ThP 026 **Enhancing drug-payload localization in antibody-drug conjugates with a middle-down approach utilizing proton transfer charge reduction on a modified Orbitrap Ascend**; Linda B Lieu<sup>1</sup>; Cynthia Nagy<sup>1</sup>; Jingjing Huang<sup>2</sup>; Christopher Mullen<sup>2</sup>; Graeme C. McAlister<sup>2</sup>; David Bergen<sup>2</sup>; Vlad Zabrouskov<sup>2</sup>; Kristina Srzentic<sup>3</sup>; Kenneth R. Durbin<sup>4</sup>; Rafael Melani<sup>2</sup>; Luca Fornelli<sup>1</sup>; <sup>1</sup>University of Oklahoma, Norman, OK; <sup>2</sup>ThermoFisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific, Reinach, Switzerland; <sup>4</sup>Proteinaceous, Inc., Evanston, IL
- ThP 027 **Platform-specific Fc N-glycan profiles of an antisperm antibody**; Ellena Nador<sup>1</sup>; Chaoshuang Xia<sup>1</sup>; Philip J. Santangelo<sup>2</sup>; Kevin J. Whaley<sup>3</sup>; Deborah J. Anderson<sup>1</sup>; Catherine E Costello<sup>1</sup>; <sup>1</sup>Boston University Chobanian & Avedisian School of Medicine, Boston, MA; <sup>2</sup>Emory University, Atlanta, GA; <sup>3</sup>ZabBio, Inc., San Diego, CA
- ThP 028 **LC-MS-based Strategy for Tissue Distribution Analysis of Antibody-Drug Conjugates in Xenograft Mice**; Bo An<sup>1</sup>; Xiaoyu Zhu<sup>1</sup>; Ming Zhang<sup>1</sup>; Jun Qu<sup>1,2</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY; <sup>2</sup>New York State Center of Excellence in Bioinformatics and Life Sciences, buffalo, New York
- ThP 029 **Studying Fab glycosylated antibody pharmacokinetics in human plasma samples at the subunit level by nano-RP-LC-MS**; Christoph Gstoettner<sup>1</sup>; Manfred Wuhrer<sup>1</sup>; Elena Dominguez Vega<sup>1</sup>; <sup>1</sup>Leiden University Medical Center, Leiden, Netherlands
- ThP 030 **Considerations for Accurate Determination of Drug-to-Antibody Ratio (DAR) of Highly-loaded Antibody Drug Conjugates (ADCs) with DAR of 8 by LC-MS**; Darby Ball<sup>1</sup>; Tahmid Hassan<sup>1</sup>; Ekaterina Deyanova<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb, Lawrence Township, NJ
- ThP 031 **LC-MS/MS and EndoS2 Workflow for Knock Out Verification of FUT8, the Gene Encoding for  $\alpha$ -(1,6) Fucosyltransferase in CHO Cells**; Benjamin Cutak<sup>1</sup>; Amber Petersen<sup>1</sup>; Andrew Feldmann<sup>1</sup>; Andrew Paoletti<sup>1</sup>; Kevin Ray<sup>1</sup>; <sup>1</sup>MilliporeSigma, Saint Louis, MO
- ThP 032 **Improved characterization of monoclonal antibodies using intact mass analysis and middle-down approaches on a modified Orbitrap Tribrid mass spectrometer**; Jingjing Huang<sup>1</sup>; Christopher Mullen<sup>1</sup>; Kristina Srzentic<sup>2</sup>; Graeme McAlister<sup>1</sup>; Vlad Zabrouskov<sup>1</sup>; Rafael Melani<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Reinach, Switzerland

### ART, ARCHAEOLOGY & PALEONTOLOGY 033-041

- ThP 033 **Low-invasive sampling method for taxonomic for the identification of archaeological and paleontological bones by proteomics of their collagens**; Isabelle Fabrizi<sup>1</sup>; Stephanie Flament<sup>1</sup>; Claire Delhon<sup>2</sup>; Lionel Gourichon<sup>2</sup>; Manon Vuillien<sup>2</sup>; Tarek Oueslati<sup>3</sup>; Patrick Auguste<sup>4</sup>; Christian ROLANDO<sup>5</sup>; Fabrice Bray<sup>5</sup>; <sup>1</sup>MSAP USR 3290, Villeneuve d'Ascq, France; <sup>2</sup>UMR 7264 - CEPAM, Nice, France; <sup>3</sup>UMR8164 - HALMA, Villeneuve d'ascq, France; <sup>4</sup>UMR 8198 - EEP, villeneuve d'ascq, France; <sup>5</sup>MSAP USR 3290, villeneuve d'ascq, France
- ThP 034 **Determination of New Biomarkers in Ceremonial Caffeinated Beverages by High-Resolution Time-of-Flight Mass Spectrometry**; Coley Beavers<sup>1</sup>; Tareq Aziz<sup>1</sup>; Adam King<sup>1</sup>; Susan D Richardson<sup>1</sup>; <sup>1</sup>University of South Carolina, Columbia, SC
- ThP 035 **Automated high-throughput biological sex identification from dental enamel using targeted proteomics**; Claire Koenig<sup>1</sup>; Patricia Bortel<sup>2</sup>; Ana Martinez-Val<sup>1</sup>; Christopher Gerner<sup>2</sup>; Fabian Kanz<sup>3</sup>; Enrico Cappellini<sup>4</sup>; Jesper Velgaard Olsen<sup>1</sup>; <sup>1</sup>Novo Nordisk Foundation Center for Protein Research (CPR), University of Copenhagen, Copenhagen, Denmark; <sup>2</sup>Department of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria; <sup>3</sup>Center for Forensic Medicine, Medical University of Vienna, Vienna, Austria; <sup>4</sup>Geogenetics Section, Globe institute, University of Copenhagen, Copenhagen, Denmark
- ThP 036 **Investigating volatilecontaminant mitigation and object cleaning methods via in-situ-SPME sampling**; Erin Birdsall<sup>1,2</sup>; G. Asher Newsome<sup>1</sup>; Susan Heald<sup>2</sup>; John George<sup>2</sup>; Gwénaëlle Kavich<sup>1</sup>; <sup>1</sup>Smithsonian Museum Conservation Institute, Suitland, MD; <sup>2</sup>Smithsonian National Museum of the American Indian, Suitland, MD
- ThP 037 **Biological Sex Estimation from Human Dental Enamel using Mass Spectrometry: Test in a Commingled Burial Context from the Iberian Peninsula**; Andrea M Zurek-Ost<sup>1</sup>; Angie L Mordant<sup>1</sup>; Allie Mills<sup>1</sup>; Thomas S Webb<sup>1</sup>; Natalie K Barker<sup>1</sup>; Emma J Bonthorne<sup>2</sup>; Laura Herring<sup>1</sup>; <sup>1</sup>University of

## THURSDAY POSTERS

- North Carolina at Chapel Hill, Chapel Hill, NC; <sup>2</sup>Aditu Arkeologia, Ubide, Spain
- ThP 038 **Collagen remains in Cretaceous fossil bone from the Isle of Wight (UK) by LC-MS;** Joseph Hubbard<sup>1</sup>; Steven Robinson<sup>2</sup>; Krzysztof Pawlak<sup>2</sup>; Stephen Taylor<sup>1</sup>; <sup>1</sup>University of Liverpool, Liverpool, United Kingdom; <sup>2</sup>Materials Innovation Factory, University of Liverpool, Liverpool, United Kingdom
- ThP 039 **First application of MALDI MSI and machine learning to historic artwork;** Václav Krupička<sup>1, 2</sup>; Florent Grélard<sup>1, 2</sup>; Landry Blanc<sup>1, 2</sup>; Julie Arslanoglu<sup>3</sup>; Aleksandra Popowich<sup>3</sup>; José Luis Lazarte<sup>4</sup>; Nicolas Desbenoit<sup>1, 2</sup>; Caroline Tokarski<sup>1, 2</sup>; <sup>1</sup>University of Bordeaux, CNRS, Bordeaux INP, CBMN, UMR 5248, Pessac, France; <sup>2</sup>Bordeaux Proteome Platform, University of Bordeaux, Bordeaux, France; <sup>3</sup>Department of Scientific Research, The Metropolitan Museum of Art, New York, NY; <sup>4</sup>Departement of Paintings Conservation, Metropolitan Museum of Art, New York, NY
- ThP 040 **Ancient Animal Diet Determined through Tandem Mass Spectrometry;** George Katselis<sup>1</sup>; Megan ME Tomilin<sup>1</sup>; Paulos Chumala<sup>1</sup>; Tina Greenfield<sup>1</sup>; <sup>1</sup>University of Saskatchewan, Saskatoon, SK
- ThP 041 **Developing untargeted and targeted proteomics methods for identification of chia oil in viceregal Mexican artworks;** Sarah E. Noll<sup>1</sup>; Aleksandra Popowich<sup>2</sup>; José Luis Lazarte<sup>3</sup>; Catherine Gilbert<sup>4, 5</sup>; Katell Bathany<sup>4, 5</sup>; Caroline Tokarski<sup>4, 5</sup>; Julie Arslanoglu<sup>1</sup>; <sup>1</sup>Department of Scientific Research, The Metropolitan Museum of Art, New York, NY; <sup>2</sup>Scientific Research Department, The Philadelphia Museum of Art, Philadelphia, PA; <sup>3</sup>Department of Paintings Conservation, The Metropolitan Museum of Art, New York, NY; <sup>4</sup>University of Bordeaux, CNRS, Bordeaux INP, CBMN, UMR 5248, Pessac, France; <sup>5</sup>Bordeaux Proteome Platform, University of Bordeaux, Bordeaux, France
- ARTIFICIAL INTELLIGENCE IN MS INSTRUMENTATION AND APPLICATIONS II**  
042-069
- ThP 042 **Advanced Stochastic Variational Inference for Accurate Constituent Estimation in Nucleic Acid Mixture Models;** Taichi Tomono<sup>1, 2, 3</sup>; Satoshi Hara<sup>1</sup>; Junko Iida<sup>3, 4</sup>; Takashi Washio<sup>1</sup>; <sup>1</sup>Department of Reasoning for Intelligence, The Institute of Scientific and Industrial Research, Osaka University, Ibaraki-shi, Japan; <sup>2</sup>AI Solution Unit, Technology Research Laboratory, Shimadzu Corporation, Soraku-gun, Japan; <sup>3</sup>Shimadzu Analytical Innovation Research Laboratories, Osaka University, Suita-shi, Japan; <sup>4</sup>Life Science Business Department, Analytical & Measuring Instruments Division, Shimadzu Corporation, Kyoto-shi, Japan
- ThP 043 **Zero-shot retention time prediction for unseen post-translational modifications with molecular structure encodings;** Ceder Dens<sup>1</sup>; Darien Yeung<sup>2</sup>; Oleg Krokhin<sup>2</sup>; Kris Laukens<sup>1</sup>; Wout Bittremieux<sup>1</sup>; <sup>1</sup>University of Antwerp, Antwerp, Belgium; <sup>2</sup>Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB
- ThP 044 **Deep Learning Models for Protein Structure Elucidation from Mass Spectrometry Data;** Steffen Lindert; *The Ohio State University, Columbus, OH*
- ThP 045 **Graphormer-IR: Fast and Accurate ML Predictions for Mass Spectrometry-measured IRMPD Spectra;** Caillum MK Stienstra<sup>1</sup>; Liam Hebert<sup>1, 2</sup>; Patrick Thomas<sup>1</sup>; Alexander Haack<sup>1, 3</sup>; W. Scott Hopkins<sup>1, 4, 5</sup>; <sup>1</sup>University of Waterloo, Waterloo, ON; <sup>2</sup>Cheriton School of Computer Science, Waterloo, ON; <sup>3</sup>Leibniz Universität Hannover, Hannover, Germany; <sup>4</sup>Watermine Innovation, Waterloo, ON; <sup>5</sup>Centre for Eye and Vision Research, Hong Kong, Hong Kong
- ThP 046 **Compression of imaging mass spectrometry datasets using convolutional autoencoders;** Zhongling Liang<sup>1</sup>; Boone M. Prentice<sup>1</sup>; <sup>1</sup>University of Florida Department of Chemistry, Gainesville, FL
- ThP 047 **UniSpec: Predicting the Full Range of Peptide Fragment Ion Series by Deep Learning Enhances Reliability in Identifying Complex Biological Peptides;** Qian Dong<sup>1</sup>; Xinjian Yan<sup>1</sup>; Joel Lapin<sup>2</sup>; <sup>1</sup>NIST, Gaithersburg, MD; <sup>2</sup>Georgetown University, Washington Dc, DC
- ThP 048 **Advanced neural network architectures for MS2 spectra encoding;** Joel Lapin<sup>1</sup>; Alfred Nilsson<sup>2</sup>; Lukas Käll<sup>2</sup>; Mathias Wilhelm<sup>1</sup>; <sup>1</sup>Computational Mass Spectrometry, TUM, Freising, Germany; <sup>2</sup>KTH Royal Institute of Technology, Stockholm, Sweden
- ThP 049 **iDeepLC: An effective retention time predictor for unseen modified peptides that can differentiate between isomers;** Alireza Nameni<sup>1, 2</sup>; Lennart Martens<sup>2, 3</sup>; Sven Degroeve<sup>1, 2</sup>; Robbin Bouwmeester<sup>2, 3</sup>; <sup>1</sup>VIB-UGent Center for Medical Biotechnology, Gent, Belgium; <sup>2</sup>Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; <sup>3</sup>VIB-UGent Center for Medical Biotechnology, Gent, Belgium
- ThP 050 **Computer Vision-Assisted Robotized Sampling of Volatile Organic Compounds;** Jing-Chi Jang<sup>1</sup>; Pawel L. Urban<sup>1</sup>; <sup>1</sup>National Tsing Hua University, Hsinchu City, Taiwan
- ThP 051 **Accounting for digestion enzyme bias in the Casanovo de novo peptide sequencing model;** Carlo F Melendez<sup>1</sup>; Justin Sanders<sup>2</sup>; Melih Yilmaz<sup>2</sup>; William S Noble<sup>1</sup>; <sup>1</sup>University of Washington - Genome Sciences, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA
- ThP 052 **Accurate prediction of antibody deamidations leveraging high-throughput automated MAM workflow, deep learning, and protein language models;** Ben Niu<sup>1</sup>; Lili Wang<sup>2</sup>; Benjamin Lee<sup>1</sup>; Wen Chen<sup>1</sup>; Henry Chan<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb, San Diego, CA; <sup>2</sup>University of California, Berkeley, Berkeley, CA
- ThP 053 **Predicting REIMS from MALDI: to prevent destruction of glioblastoma sections used for model improvement;** Thomas Vanhemel<sup>1</sup>; Melanie Nijs<sup>1</sup>; Angeliki Birmpilii<sup>2</sup>; Tim Hendriks<sup>2</sup>; Eva Cuypers<sup>2</sup>; Bart De Moor<sup>1</sup>; <sup>1</sup>KU Leuven, ESAT-STADIUS, Leuven, Belgium; <sup>2</sup>Maastricht University, Maastricht, Netherlands
- ThP 054 **Metabolomics with absolute concentrations but without calibration curves or isotopologues: extension of AI model to instruments not used in training;** Ana S.H. Costa<sup>1</sup>; Bashar Amer<sup>2</sup>; Rahul R. Deshpande<sup>2</sup>; Luke S. Ferro<sup>1</sup>; Jack Howland<sup>1</sup>; Joshua D. Lauterbach<sup>1</sup>; Jefferson G. Pruyne<sup>1</sup>; Devesh Shah<sup>1</sup>; Timothy Kassis<sup>1</sup>; Susan S Bird<sup>2</sup>; Jennifer M Campbell<sup>1</sup>; <sup>1</sup>Matterworks, Somerville, MA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 055 **Improved de novo peptide sequencing with higher quality training data;** Melih Yilmaz<sup>1</sup>; William E Fondrie<sup>2</sup>; Wout Bittremieux<sup>3</sup>; Carlo F Melendez<sup>1</sup>; Varun Ananth<sup>1</sup>; Sewoong Oh<sup>1</sup>; William S Noble<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Talus Bioscience, Seattle, WA; <sup>3</sup>University of Antwerp, Antwerp, Belgium
- ThP 056 **Enhancing Protein-Based Human Identification Using AI-Extended Mass Spectral Libraries;** Douglas Slotta<sup>1</sup>; Zachary C Goecker<sup>1</sup>; Lewis Y. Geer<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD
- ThP 057 **LSM1-MS2: A self-supervised foundation model for MS2 downstream tasks including broad chemical property prediction and spectral lookup;** Gabriel Asher<sup>1</sup>; Jennifer M Campbell<sup>1</sup>; Jack Geremia<sup>1</sup>; Timothy Kassis<sup>1</sup>; <sup>1</sup>Matterworks, Inc., Somerville, MA
- ThP 058 **A Bayesian model for estimating the posterior error probability and the false discovery rate of de novo peptide sequencing;** Ngoc Hieu Tran<sup>1</sup>; Rui Qiao<sup>1</sup>; Lei Xin<sup>1</sup>; Baozhen Shan<sup>1</sup>; <sup>1</sup>Bioinformatics Solutions Inc, Waterloo, ON
- ThP 059 **Benchmarking machine learning strategies for phosphoproteomic data in clear cell renal carcinoma diagnosis and staging;** Nazrath Nawaz<sup>1</sup>; Weronika E. Borek<sup>1</sup>; Josie A. Christopher<sup>1</sup>; Pedro Moreno-Cardoso<sup>1</sup>; David N. Perkins<sup>1</sup>; Amy E. Campbell<sup>1</sup>; Pedro R. Cutillas<sup>1, 2</sup>; Arran D. Dokal<sup>1</sup>; <sup>1</sup>Kinomic Ltd, Macclesfield, Cheshire, United Kingdom; <sup>2</sup>Barts Cancer Institute, Queen Mary University of London, London, United Kingdom
- ThP 060 **Breaking Barriers in Complex Sample Analysis: Predicting Total Acid Number and Sulfur Content**

## THURSDAY POSTERS

- through FT-ICR-MS Data with Machine Learning Approaches; Jussara Valente Roque<sup>1</sup>; Wilson Junior Cardoso<sup>2</sup>; Gesiane da Silva Lima<sup>2</sup>; Gabriel Franco Dos Santos<sup>2</sup>; Alexandre de Oliveira Gomes<sup>3</sup>; Iris Medeiros Junior<sup>3</sup>; Boniek Gontijo Vaz<sup>2</sup>; <sup>1</sup>Universidade Federal de Goiás, Goiânia, Brazil; <sup>2</sup>Universidade Federal de Goiás, Goiânia, Brazil; <sup>3</sup>PETROBRAS, Rio de Janeiro, Brazil
- ThP 061 **A learned score function improves the power of mass spectrometry database search;** Varun R Ananth<sup>1</sup>; Justin Sanders<sup>1</sup>; Melih Yilmaz<sup>1</sup>; Sewoong Oh<sup>1</sup>; William S Noble<sup>1,2</sup>; <sup>1</sup>Paul G. Allen School of Computer Science and Engineering, University of Washington, Seattle, WA; <sup>2</sup>University of Washington - Genome Sciences, Seattle, WA
- ThP 062 **MassQL Assistant - A Custom GPT4 Assistant To Enhance Accessibility to Query Mass Spectrometry Data with MassQL;** Kartik Gulia<sup>1</sup>; Mingxun Wang<sup>1</sup>; <sup>1</sup>University of California Riverside, Riverside, CA
- ThP 063 **GraphOmicsNet: a unified pipeline of integrated cancer omics with graph autoencoder for molecular classification of cancers;** Yiyang Chen<sup>1,2</sup>; Guixue Hou<sup>1,2</sup>; Siqi Liu<sup>1,2</sup>; <sup>1</sup>University of Chinese Academy of Sciences, Beijing, China; <sup>2</sup>BGI, Shenzhen, China
- ThP 064 **Artificially Intelligent copilot for Automating LC-OzESI-MRM Lipidomics Experiments and Analysis using Large Language Models;** Sanjay Iyer<sup>1</sup>; Caitlin E. Randolph<sup>2</sup>; Matthew Muhoberac<sup>2</sup>; Connor Beveridge<sup>2</sup>; Shane Tichy<sup>3</sup>; Gaurav Chopra<sup>2,4,5,6,7,8,9</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Purdue University, Department of Chemistry, West Lafayette, IN; <sup>3</sup>Agilent Technologies, Santa Clara, CA; <sup>4</sup>Purdue University, Department of Computer Science, West Lafayette, IN; <sup>5</sup>Purdue Institute for Drug Discovery, West Lafayette, IN; <sup>6</sup>Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; <sup>7</sup>Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; <sup>8</sup>Purdue Institute for Integrative Neuroscience, West Lafayette, IN; <sup>9</sup>Regenstrief Center for Healthcare Engineering, West Lafayette, IN
- ThP 065 **Predicting compositional fragments of compounds from their tandem mass spectra using deep neural networks;** Yuhui Hong<sup>1</sup>; Sujun Li<sup>1,2</sup>; Yuzhen Ye<sup>1</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>GlycoMS LLC, Bloomington, IN
- ThP 066 **Benchmarking prediction models for improved peptide identification with MSBooster and FragPipe;** Kevin L Yang<sup>1</sup>; Fengchao Yu<sup>1</sup>; Ludwig Lautenbacher<sup>2</sup>; Mathias Wilhelm<sup>2</sup>; Alexey I Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, Michigan; <sup>2</sup>Computational Mass Spectrometry, TUM, Freising, Germany
- ThP 067 **Automatic Registration of MALDI images with Atlases;** Pasindu Tennakoon<sup>1</sup>; Pulasthi Ekanayake<sup>1</sup>; Sanoj Silva<sup>1</sup>; Lalin Theverapperuma<sup>1</sup>; Andi Krupke<sup>1</sup>; <sup>1</sup>Expert Intelligence, Santa Clara, CA
- ThP 068 **Exploring the Future of MS: AI-Guided Design of MALDI Matrices using Theoretical and Empirical Insights;** Carlos A. Padilla<sup>1</sup>; Emmanuel Campo<sup>2</sup>; Luis M. Díaz-Sánchez<sup>1</sup>; Cristian Blanco-Tirado<sup>1</sup>; Aldo F. Combariza<sup>2</sup>; Marianny Y. Combariza<sup>1</sup>; <sup>1</sup>Universidad Industrial de Santander, Bucaramanga, Colombia; <sup>2</sup>Universidad de Sucre, Sincelejo, Colombia
- ThP 069 **Artificially Intelligent copilot for Automating Lipidomics Experiments and Analysis using Large Language Models;** Connor H Beveridge<sup>1</sup>; Matthew Muhoberac<sup>1</sup>; Sanjay Iyer<sup>1</sup>; Caitlin Randolph<sup>1</sup>; Palak Manchanda<sup>1</sup>; Shane Tichy<sup>2</sup>; Gaurav Chopra<sup>3,4,5,6,7,8,9</sup>; <sup>1</sup>Purdue University Department of Chemistry, West Lafayette, IN; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>Purdue University, Department of Chemistry, West Lafayette, IN; <sup>4</sup>Regenstrief Center for Healthcare Engineering, West Lafayette, IN; <sup>5</sup>Purdue Institute for Drug Discovery, West Lafayette, IN; <sup>6</sup>Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; <sup>7</sup>Purdue Institute for Integrative Neuroscience, West Lafayette, IN; <sup>8</sup>Purdue University, Department of Computer Science, West Lafayette, IN;
- <sup>9</sup>Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN
- BIOMARKERS: DISCOVERY II**  
**070-079**
- ThP 070 **EAD-enabled intact glycopeptide/glycoproteome characterization for site-specific glycoproteomics;** Zhengwei Chen<sup>1</sup>; Lei Xiong<sup>2</sup>; <sup>1</sup>SCIEX, Redwood city, CA; <sup>2</sup>SCIEX, Redwood City, CA
- ThP 071 **Integration of metabolic pathway and network analysis for discovering the biomarkers of fruit-vegetable intervention in pig feces;** Zhihao Liu<sup>1</sup>; Gloria Solano-Aguilar<sup>1</sup>; Sukla Lakshman<sup>1</sup>; Joseph F. Urban<sup>1</sup>; Mengliang Zhang<sup>2</sup>; Pei Chen<sup>1</sup>; Liangli Yu<sup>3</sup>; Jianghao Sun<sup>1</sup>; <sup>1</sup>USDA-ARS, Beltsville, MD; <sup>2</sup>Middle Tennessee State University, Murfreesboro, TN; <sup>3</sup>University of Maryland, College Park, College park, MD
- ThP 072 **Identification of a Lactosylceramide Phosphate as Biomarker for Niemann Pick Disease Type C1;** Sonali Mishra<sup>1</sup>; Pamela Kell<sup>1</sup>; Xuntian Jiang<sup>1</sup>; Dennis J. Dietzen<sup>1</sup>; Charles H. Vite<sup>2</sup>; Elizabeth Berry-Kravis<sup>3</sup>; Stephanie M. Cologna<sup>4</sup>; Forbes D. Porter<sup>5</sup>; <sup>1</sup>Washington University school of Medicine, St Louis, MO; <sup>2</sup>University of Pennsylvania School of Veterinary Medicine, Pennsylvania, PA; <sup>3</sup>Rush University Medical Center, Chicago, IL; <sup>4</sup>University of Illinois Chicago, Chicago, IL; <sup>5</sup>Arbor Biotechnologies, Cambridge, MA
- ThP 073 **Identification of Biomarkers for Early Detection of Small Cell Lung Cancer Using LC-MS;** Kinnari Chaubal<sup>1</sup>; Yue Li<sup>2</sup>; <sup>1</sup>Thomas Jefferson High School for Science and Technology, Alexandria, VA; <sup>2</sup>University of Maryland, College Park, College park, MD
- ThP 074 **Decoding Cellular Signatures: Mass Spectrometry Analysis of Exosomes and Total Cellular Proteins from Human Astrocytes and Endothelial Brain Cells;** Kristen H. Hutson<sup>1</sup>; Guoting Qin<sup>2</sup>; Chengzhi Cai<sup>3</sup>; Gergana G. Nestorova<sup>4</sup>; Guoting Qin<sup>2</sup>; <sup>1</sup>Ph.D. student, Molecular Science and Nanotechnology, Louisiana Tech University, Ruston, LA; <sup>2</sup>Research Associate Professor, College of Optometry, University of Houston, Houston, Texas; <sup>3</sup>Professor, Department of Chemistry, University of Houston, Houston, Texas; <sup>4</sup>Associate Professor, School of Biological Sciences, Louisiana Tech University, Ruston, LA
- ThP 075 **Investigating the Dynamics of the Proteome in the Cerebellum of the Neurodegenerative NPC1 mice model;** Varshasnata Mohanty<sup>1</sup>; Wenping Li<sup>1</sup>; Stephanie M Cologna<sup>1</sup>; <sup>1</sup>University of Illinois at Chicago, Chicago, IL
- ThP 076 **A Rapid and Economical Workflow to Discover Protein Biomarkers Using High-performance Triple Quadrupole LC/MS System;** Lin Feng Wu<sup>1</sup>; Ian Edwards<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- ThP 077 **Optimisation of ZenoSWATH DIA workflows for higher throughput plasma protein relative quantification;** Haneen Alharbi<sup>1</sup>; Richard Unwin<sup>1</sup>; <sup>1</sup>The University of Manchester, Manchester, United Kingdom
- ThP 078 **Reproducibility-optimized multi-group statistic and survival analysis;** Markus Linden<sup>1</sup>; Laura L. Elo<sup>1</sup>; Tommi Suomi<sup>1</sup>; <sup>1</sup>University of Turku, Turku, Finland
- ThP 079 **Unique high-throughput workflow for deeper plasma/serum proteome coverage enables discovery of novel biomarkers;** Measho Abreha<sup>1</sup>; Katharina Limm<sup>2</sup>; Zehan Hu<sup>2</sup>; Katrin Hartinger<sup>2</sup>; Andreas Schmidt<sup>3</sup>; Sebastian Mueller<sup>4</sup>; Nils A. Kulak<sup>2</sup>; <sup>1</sup>PreOmics, Billerica, MA; <sup>2</sup>PreOmics, Planegg/Martinsried, Germany; <sup>3</sup>Bruker Daltonics GmbH & Co.KG, Bremen, Germany; <sup>4</sup>Biognosys AG, Zuerich, Switzerland
- ThP 080 **Overcoming the dynamic range difficulties in CSF samples through a novel enrichment step for biomarker discovery studies;** Katharina Limm<sup>1</sup>; Zuzana Demianova<sup>1</sup>; Katrin Hartinger<sup>1</sup>; Nils A. Kulak<sup>2</sup>; <sup>1</sup>PreOmics, Planegg/Martinsried, Germany
- ThP 081 **Deep proteome profiling of Cynomolgus monkey Cerebrospinal Fluid by LCMS;** Xuemei Yang<sup>1</sup>; Youhei



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- Kosugi<sup>1</sup>; Tomoki Yamashita<sup>1</sup>; Faizan Zubair<sup>1</sup>; <sup>1</sup>Takeda, Cambridge, MA
- ThP 082 **Comparison of Different Collection Methodologies for the Proteomic Analysis of Tear Fluid;** Campbell B Mousseau<sup>1, 2</sup>; Nicole M Schaeublin<sup>1, 2</sup>; Alena R Veigl<sup>1, 2</sup>; Rhonda L Pitsch<sup>2</sup>; Sean W Harshman<sup>2</sup>; <sup>1</sup>UES, Inc. - an eclipse company, Dayton, OH; <sup>2</sup>Air Force Research Laboratory, Aerospace Systems Directorate, Dayton, OH
- ThP 083 **Identification of Biomarkers in Cerebrospinal Fluid of Schizophrenia Rat Model;** Shideh Mirhadi<sup>1</sup>; Carlo P. Ramil<sup>1</sup>; Mackenzie Hoffmann<sup>2</sup>; Xiaohai Wang<sup>2</sup>; An Chi<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., Cambridge, MA; <sup>2</sup>Merck & Co. Inc., West Point, PA
- ThP 084 **Discovery of metabolite biomarkers of primary headaches with mass spectrometry-based metabolomics;** Shen Hu; UCLA, Los Angeles, CA
- ThP 085 **Uncovering more biological insights in your samples with routine LC/Q-TOF workflows for metabolites and lipids;** Karen Yannell<sup>1</sup>; Cate Simmermaker<sup>1</sup>; Sierra D. Durham<sup>1</sup>; Genevieve Van De Bittner<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- ThP 086 **An amino-rich polymer-coated magnetic nanomaterial for ultra-rapid separation of phosphorylated peptides in the serum of Parkinson's disease patients;** Chuan-Fan Ding<sup>1</sup>; Yinghua Yan<sup>1</sup>; <sup>1</sup>Ningbo University, Ningbo, China
- ThP 087 **Comprehensive TMTpro-16plex based plasma proteome profiling of non-human primate plasma to discover biomarkers for radiation-induced injury;** Mehari Weldemariam<sup>1</sup>; Christina Williams<sup>1</sup>; Maureen A. Kane<sup>1</sup>; <sup>1</sup>University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, Maryland
- ThP 088 **GlycoISA – Combining Immunosorbent Assay with LC-MS/MS for Glycoproteomic Analysis of Antigen-Specific Antibodies;** Yiyun Liu<sup>1</sup>; Armin Oloumi<sup>1</sup>; Antonio Ji-Xu<sup>1</sup>; Diane Dayoung Park<sup>1</sup>; Ron Feldman<sup>2</sup>; Emanuel Maverakis<sup>1</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA; <sup>2</sup>Emory University School of Medicine, Atlanta, GA
- ThP 089 **Dia-PASEF for in-depth immunopeptidomics analysis: Challenges and new opportunities;** Kristina Marx<sup>1</sup>; Naomi Hoenisch Gravel<sup>2, 3, 4</sup>; Torsten Mueller<sup>1</sup>; Pierre-Olivier Schmit<sup>1</sup>; Daniel Hornburg<sup>5</sup>; Juliane Walz<sup>2, 3, 4, 6</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; <sup>2</sup>Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tübingen, Tübingen, Germany; <sup>3</sup>Cluster of Excellence iFIT (ECX2180) "Image-Guided and Functionally Instructed Tumor Therapies"; University of Tuebingen, Tuebingen, Germany; <sup>4</sup>Institute for Cell Biology, Department of Immunology, University of Tuebingen, Tuebingen, Germany; <sup>5</sup>Bruker Scientific, 40 Manning Road, Billerica, MA; <sup>6</sup>Clinical Collaboration Unit Translational Immunology, Department of Internal Medicine, University Hospital Tuebingen, Tuebingen, Germany
- ThP 090 **Evaluating biofluid biomarker potential of the healthy feline proteome in urine, plasma, and serum;** Katelyn B Brusach<sup>1</sup>; Ariana E Shannon<sup>1</sup>; Brian C Searle<sup>1</sup>; Jessica M Quimby<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH
- ThP 091 **Development of red blood cells and plasma-based diagnostic lipid biomarker panel for Parkinson's disease;** Fathima Shaima MuhammedNazaar<sup>1</sup>; Anne M Roberts<sup>1</sup>; Ankit Jain<sup>1</sup>; James Doecke<sup>2</sup>; Malcolm Horne<sup>3</sup>; Stephan Klatt<sup>4</sup>; Blaine Roberts<sup>1</sup>; <sup>1</sup>Emory University, Atlanta, GA; <sup>2</sup>CSIRO Health and Biosecurity, Herston, Australia; <sup>3</sup>The Florey Institute of Neuroscience and Mental Health, The University of Melbourne, Parkville, Australia; <sup>4</sup>Institute for Vascular Signaling, Center for Molecular Medicine, Goethe University, 60590, Germany
- ThP 092 **Proteomic Analysis of Aqueous Humor Biomarkers Associated with Neovascular Complications in Diabetic Retinopathy;** Jaewon Oh<sup>1</sup>; Seong Joon Ahn<sup>2</sup>; Jae Hun Jung<sup>1</sup>; Tae Wan Kim<sup>3</sup>; Kwang Pyo Kim<sup>1</sup>; <sup>1</sup>Kyung-Hee University, Yong-in, South Korea; <sup>2</sup>Hanyang University College of Medicine, Seoul, South Korea; <sup>3</sup>SNU, Seoul, South Korea
- ThP 093 **Deciphering Immune Profiles and Proteomic Signatures Correlated with Fusobacterium nucleatum in Colorectal Cancer;** Qiangmin Zhang<sup>1</sup>; Xi Peng<sup>1</sup>; Hyun Young Park<sup>1</sup>; Rosie Blodgett<sup>1</sup>; Patrick Wagner<sup>1</sup>; Kevin (Kunhong) Xiao<sup>1</sup>; <sup>1</sup>AHN, Pittsburgh, PA
- ThP 094 **Global Proteomics Identifies CDK11 and Spliceosome SF3B1 as Integral to Myeloma Proliferation and High-Risk Disease;** David E Mery<sup>1</sup>; Visanu Wanchai<sup>1</sup>; Timothy Cody Ashby<sup>1</sup>; Samuil Ivanovsky<sup>1</sup>; Hongwei Xu<sup>1</sup>; Eric Siegel<sup>1</sup>; Clyde Bailey<sup>1</sup>; Sandra G Mattox<sup>1</sup>; Samer Al Hadidi<sup>1</sup>; Carolina D Schinke<sup>1</sup>; Sharmilan Thanendrarajan<sup>1</sup>; Maurizio Zangari<sup>1</sup>; Frits Van Rhee<sup>1</sup>; Guido J Tricot<sup>1</sup>; John D Shaughnessy Jr<sup>1</sup>; Fenghuang Zhan<sup>1</sup>; <sup>1</sup>UAMS, Little Rock, AR
- ThP 095 **Charting the metabolic biogeography of the colorectum in cancer: challenging the proximal versus distal classification;** Abhishek Jain<sup>1</sup>; Caroline Johnson<sup>1</sup>; Sajid A. Khan<sup>2</sup>; Montana T. Morris<sup>2</sup>; Domenica Berardi<sup>1</sup>; Jason Crawford<sup>2</sup>; Noah Palm<sup>2</sup>; Deguang Song<sup>2</sup>; <sup>1</sup>Yale School of Public Health, New Haven, CT; <sup>2</sup>Yale School of Medicine, New Haven, CT
- ThP 096 **Adaptation of plasma-enrichment strategies for fast and sensitive analysis of cerebrospinal fluid;** Eva Borràs<sup>1, 2</sup>; Federica Anastasi<sup>3, 4, 5</sup>; Olga Pastor<sup>1, 2</sup>; Marc Suarez-Calvet<sup>3, 4, 5</sup>; Eduard Sabido<sup>1, 2</sup>; <sup>1</sup>Universitat Pompeu Fabra, Barcelona, Spain; <sup>2</sup>Centre for Genomic Regulation, Barcelona, Spain; <sup>3</sup>BarcelonaBeta Brain Research Center, Barcelona, Spain; <sup>4</sup>Pasqual Maragall Foundation, Barcelona, Spain; <sup>5</sup>Hospital del Mar Research Institute, Barcelona, Spain
- ThP 097 **Advancing Tear Fluid Proteomics: Optimization of LC-MS/MS Protocol for Enhanced Analysis;** James Xiao<sup>1</sup>; Sally Fu<sup>1</sup>; Kyla Frenia<sup>1</sup>; Jackie Sikora<sup>1</sup>; Leanne Labriola<sup>1</sup>; <sup>1</sup>Innsight Technology, INC., Pittsburgh, PA
- ThP 098 **Alterations in tear proteomes of adults with pre-diabetes and type 2 diabetes mellitus but without diabetic retinopathy;** Guoting Qin<sup>1</sup>; Cecilia Chao<sup>1, 2</sup>; Shara Duong<sup>1</sup>; Jennyfer Smith<sup>1</sup>; Hong Lin<sup>3</sup>; Jennifer Copeland<sup>4</sup>; Huamin Cai<sup>4</sup>; Stan Stearns<sup>4</sup>; Kathryn Richdale<sup>1</sup>; Wendy Harrison<sup>1</sup>; Chengzhi Cai<sup>1</sup>; <sup>1</sup>University of Houston, Houston, TX; <sup>2</sup>University of New South Wales, Sydney, Australia; <sup>3</sup>University of Houston-Downtown, Houston, TX; <sup>4</sup>VICI Valco Instruments, Houston, TX
- ThP 099 **Proteome Analysis of Isolated Exosomes from Control and Toxicant-Exposed Bronchoalveolar Lavage Fluids;** Zachary Hutchins<sup>1</sup>; Yinsheng Wang<sup>2</sup>; Andrea Adamcakova-Dodd<sup>3</sup>; Abu Ebrahim Siddique<sup>3</sup>; <sup>1</sup>University of California, Riverside, Redlands, CA; <sup>2</sup>University of California, Riverside, Riverside, CA; <sup>3</sup>University of Iowa, Iowa City, IA

### BIOMARKERS: QUANTITATIVE ANALYSIS III 100-126

- ThP 100 **Validated Biomarker Assay for the Analysis of Coproporphyrin I and Coproporphyrin III in Human Plasma;** Shane Karnik<sup>1</sup>; John Begley<sup>1</sup>; Benjamin Begley<sup>1</sup>; Davonne J Auguste<sup>1</sup>; Mathew Begley<sup>1</sup>; <sup>1</sup>Aliri Bioanalysis, COLORADO SPGS, CO
- ThP 101 **Comparative Analysis of Skyline and SmartPeak Performance in Quantifying a 60-Biomarker Panel in Plasma from Inflammatory Bowel Disease Patients;** Dragana Noe<sup>1</sup>; Chi D. L. Nguyen<sup>1</sup>; Erika Hernandez<sup>1</sup>; Jonathan T. Bui<sup>1</sup>; Jennifer E. Van Eyk<sup>2</sup>; Susan M. Mockus<sup>1</sup>; <sup>1</sup>Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA; <sup>2</sup>Advanced Clinical BioSystems Research Institute, Cedars-Sinai Medical Center, Los Angeles, CA
- ThP 102 **LC-MS/MS Method Development of Endogenous Small Molecule Biomarker: Case Studies;** Jingguo Hou<sup>1</sup>; Xiaodong Zhu<sup>1</sup>; Sarah Garcia<sup>1</sup>; Steven Hoehne<sup>1</sup>; Xiaomei Bian<sup>1</sup>; Leimin Fan<sup>1</sup>; <sup>1</sup>Worldwide Clinical Trials, Austin, TX
- ThP 103 **A Fully Validated Automated Method for the Detection of Cotinine and Hydroxycotinine in Human Serum: Hamilton Vantage™ and LC/MS/MS;** Danielle L Sowle<sup>1</sup>;

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- Tiffany Seyler<sup>1</sup>; Madeline Weaver<sup>2</sup>; Lanqing Wang<sup>1</sup>; <sup>1</sup>CDC, Atlanta, GA; <sup>2</sup>Oak Ridge Institute for Science and Education, Oak Ridge, TN
- ThP 104 **An ultra-sensitive technique for absolute, accurate quantification of FcRn and FcγRs on plasma-membrane and cellular-levels across different human cell types;** Qingqing Shen<sup>1, 2</sup>; Chao Xue<sup>1, 2</sup>; Xiaoyu Zhu<sup>1, 2</sup>; Jun Qu<sup>1, 2</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY; <sup>2</sup>New York State Center of Excellence in Bioinformatics and Life Sciences, buffalo, New York
- ThP 105 **Quantification of plakophilin 2A in human heart by high resolution mass spectrometry;** Kevin P. Gillespie<sup>1</sup>; Clementina Mesaros<sup>1</sup>; Ian Alexander Blair<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA
- ThP 106 **Integrated Assay Development Platform for in vivo Target Detection in Support of Drug Discovery;** Jingjing Deng<sup>1</sup>; Bogdan Slecza<sup>1</sup>; Josh Nicklay<sup>1</sup>; Eugene Ciccimaro<sup>1</sup>; Petia Shipkova<sup>1</sup>; <sup>1</sup>BMS, Princeton, NJ
- ThP 107 **Facilitating precision medicine through targeted proteomics analysis of dried plasma from fingerpricks;** Andreas Hober<sup>1</sup>; Marcus Henricsson<sup>1</sup>; Remco Van Soest<sup>2</sup>; Sahana Mollah<sup>2</sup>; Patrick Pribil<sup>3</sup>; Tasso Miliotis<sup>1</sup>; <sup>1</sup>AstraZeneca, Mölndal, Sweden; <sup>2</sup>SCIEX, Redwood City, CA; <sup>3</sup>SCIEX, Concord, ON
- ThP 108 **Unveiling Hidden Depths: A High-Throughput Plasma Proteomics Workflow for Enhanced Biomarker Discovery on Orbitrap Astral Mass Spectrometer;** Kevin Yang<sup>1</sup>; Nicholas Mucci<sup>2</sup>; Evangelina Bahu<sup>2</sup>; Andrea Cerda<sup>2</sup>; Lee Cantrell<sup>2</sup>; Khatereh Motamedchaboki<sup>1</sup>; Stephanie Samra<sup>1</sup>; Amirmansoor Hakimi<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Seer Inc., Redwood City, CA
- ThP 109 **Development of Isobaric Peptide Probes for Multiplex Disease Detection using Mass Spectrometry-Based Immunoassay;** Stephanee Joy B Zerrudo<sup>1</sup>; Ayesha Seth<sup>1</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH
- ThP 110 **Know Your Proteome: Exploring personalized proteomics in precision health;** Felicia K Ooi<sup>1</sup>; Monica Ghaly<sup>1</sup>; Santosh D Bhosale<sup>1</sup>; Stephen A. Whelan<sup>1</sup>; Susan M Mockus<sup>1</sup>; <sup>1</sup>Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA
- ThP 111 **Development and Optimization of a LC-MS/MS Method for Accurate Quantification of NAD<sup>+</sup> and NAADP Dinucleotides;** Elias Beretta<sup>1</sup>; Yongjin Yao<sup>1</sup>; Danielle Tonev<sup>1</sup>; Purvi Jejurkar<sup>1</sup>; AbbVie, South San Francisco, CA
- ThP 112 **Low-pg/mL quantitation of leucine-rich repeat kinase 2 (LRRK2) using LC-MS/MS in human cerebrospinal fluid (CSF);** Jason Causon<sup>1</sup>; Dylan Bennett<sup>2</sup>; Arash Rassoulpour<sup>2</sup>; Rahul Baghla<sup>3</sup>; <sup>1</sup>SCIEX, Framingham; <sup>2</sup>Neuron23, South San Francisco, CA; <sup>3</sup>SCIEX, Redwood City, CA
- ThP 113 **A CLIA Accredited, GCP-Compliant, high-throughput LC-MS/MS Method for Quantification of Phenylalanine and Tyrosine in Human K2EDTA Plasma;** Nicole Boone<sup>1</sup>; Tian-Sheng Lu<sup>1</sup>; Shuyu Hou<sup>1</sup>; <sup>1</sup>Medpace, Cincinnati, OH
- ThP 114 **The combination of pharmacokinetic studies and targeted metabolomics as a powerful tool for identifying exposure biomarkers of apple intake;** Shengmin Sang<sup>1</sup>; Junhe Yu<sup>1</sup>; Weixin Wang<sup>1</sup>; Yingdong Zhu<sup>1</sup>; <sup>1</sup>North Carolina A&T State University, Kannapolis, NC
- ThP 115 **Development of highly sensitive mass spectrometry methods for phosphorylated protein analysis;** Siqi Li<sup>1</sup>; Wayne Leifert<sup>2, 3</sup>; Tara Pukala<sup>1</sup>; <sup>1</sup>University of Adelaide, School of Physics, Chemistry and Earth Sciences, Adelaide, Australia; <sup>2</sup>University of Adelaide, School of Biological Sciences, Adelaide, Australia; <sup>3</sup>CSIRO Health and Biosecurity, Adelaide, Australia
- ThP 116 **An LC-MS/MS Method for Detection of a Panel of Steroids Related to The Hypertension for In Vivo Samples;** Hongfang Cui<sup>1</sup>; Hongmei Wang<sup>1</sup>; Hefeng Zhang<sup>1</sup>; Zhiren Yu<sup>1</sup>; Nan Zhao<sup>1</sup>; Zhiyu Li<sup>1</sup>; Lili Xing<sup>1</sup>; Yi Tao<sup>1</sup>; Liang Shen<sup>1</sup>; <sup>1</sup>WuXi AppTec, Shanghai, China
- ThP 117 **An LC-MS/MS method for the determination of tetrodotoxin (TTX) in SLC transporters;** Lingyan Hua<sup>1</sup>; Dan Li<sup>1</sup>; Yangzhen Zheng<sup>1</sup>; Jinlian Lu<sup>1</sup>; Zhiyu Li<sup>1</sup>; Lili Xing<sup>1</sup>; Yi Tao<sup>1</sup>; Liang Shen<sup>1</sup>; <sup>1</sup>WuXi AppTec, Shanghai, China
- ThP 118 **PRM method development for lung cancer patient classification integrated into a clinical decision support system, the Molecular Tumor Board Portal;** Georgios Mermelekas<sup>1</sup>; Olena Berkovska<sup>1</sup>; David Tamborero<sup>1</sup>; Lukas Orre<sup>1</sup>; Janne Lehtio<sup>1</sup>; <sup>1</sup>Karolinska Institutet, Solna, Sweden
- ThP 119 **Proteverse™; an easy-accessible and interactive web interface to help users generate insights into their proteomics data;** Patrick Vanzalm; <sup>1</sup>Biognosys, Zurich, Switzerland
- ThP 120 **FAIMS-PRM quantification of amol levels of STEAP2 from laser-microdissected human tissues confirms low non-prostate levels, resolving immunohistochemistry-based data concerns;** Steve M Sweet<sup>1</sup>; Jenn Morris<sup>1</sup>; Kenesha Riley<sup>1</sup>; Clare Hoover<sup>2</sup>; Deborah Berry<sup>1</sup>; David Chain<sup>1</sup>; Yeoun Jin Kim<sup>1</sup>; <sup>1</sup>AstraZeneca, Gaithersburg, MD; <sup>2</sup>AstraZeneca, Waltham, MA
- ThP 121 **Identification and quantification of phospholipids in contact lens deposits;** Mengyu Xu<sup>1</sup>; Fang Lu<sup>1</sup>; <sup>1</sup>Johnson & Johnson Vision, Jacksonville, Florida
- ThP 122 **Empowering Translational Research: High-Throughput Plasma Proteomics for Precision Medicine on Orbitrap Exploris 480 Mass Spectrometer;** Kevin Yang<sup>1</sup>; Nicholas Mucci<sup>2</sup>; Evangelina Bahu<sup>2</sup>; Andrea Cerda<sup>2</sup>; Lee Cantrell<sup>2</sup>; Khatereh Motamedchaboki<sup>1</sup>; Stephanie Samra<sup>1</sup>; Amirmansoor Hakimi<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Seer Inc., Redwood City, CA
- ThP 123 **Characterization of MUC5AC and MUC5B in sputum from patients with a respiratory disease using a qualified high-throughput LC-MS/MS method;** Monika Mital Kansal<sup>1</sup>; Anna Chen Guttman<sup>1</sup>; John-Paul Oliveria<sup>1</sup>; William Rodney Mathews<sup>1</sup>; Michele A. Grimaldeston<sup>1</sup>; Veronica Anania<sup>1</sup>; <sup>1</sup>Genentech Inc, South San Francisco, CA
- ThP 124 **Multi-OMICS biosignature phenotype stratification analysis for monitoring personal health optimization;** Stephen A. Whelan<sup>1</sup>; Felicia K Ooi<sup>1</sup>; Nathan Hendricks<sup>1</sup>; Dragana Noe<sup>1</sup>; Susan M. Mockus<sup>1</sup>; <sup>1</sup>Cedars-Sinai Precision Biomarker Labs (PBL), Beverly Hills, CA
- ThP 125 **A Sensitive and Simple LC-MS/MS Method for Simultaneous Determination of GABA and GHB in Plasma;** Haiyan Li<sup>1</sup>; Cheng Chen<sup>1</sup>; Meijuan He<sup>1</sup>; Xinxin Wen<sup>1</sup>; Xiaotong Li<sup>1</sup>; Zhiyu Li<sup>1</sup>; Lili Xing<sup>1</sup>; Yi Tao<sup>1</sup>; Liang Shen<sup>1</sup>; <sup>1</sup>WuXi AppTec, Shanghai, China
- ThP 126 **Liquid Chromatography and Tandem Mass Spectrometry for Quantitation of Endogenous Enantiomers of 3-Hydroxybutyric Acid in Dog Plasma;** Na Li<sup>1</sup>; Li Gao<sup>1</sup>; Yanfu Ren<sup>1</sup>; Zhiyu Li<sup>2</sup>; Lili Xing<sup>2</sup>; Yi Tao<sup>2</sup>; Liang Shen<sup>2</sup>; <sup>1</sup>WuXi AppTec, Suzhou, China; <sup>2</sup>WuXi AppTec, Shanghai, China

### CANCER RESEARCH II 127-160

- ThP 127 **Mass spectrometry-based analysis of proteins and intact glycopeptides in patient urine samples reveals differences associated with prostate cancer;** Nikhiya Shamsheer<sup>1</sup>; Fernando Garcia-Marques<sup>1</sup>; Abel Bermudez<sup>1</sup>; Mark R Flory<sup>2</sup>; Sharon J Pitteri<sup>1</sup>; <sup>1</sup>Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; <sup>2</sup>Cancer Early Detection Advanced Research (CEDAR) Center, Knight Cancer Institute, Oregon Health & Science University, Portland, OR
- ThP 128 **NanoLC-MS/MS DIA Unveils Unfolded-Protein-Response Landscape in Glioma: Illuminating PERK Branch Influence on Lysosomal Dynamics and Ganglioside Fluctuation;** Alexander Wenger<sup>1</sup>; Emma Phillips<sup>2</sup>; Chi D. L. Nguyen<sup>3</sup>; Violaine Rosenstiel-Goidts<sup>2</sup>; Robert Ahrends<sup>1, 3</sup>; <sup>1</sup>University of Vienna / Department of Chemistry / Institute of Analytical Chemistry, Vienna, Austria; <sup>2</sup>DKFZ German Cancer Research Center, Heidelberg,

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- Germany; <sup>3</sup>Leibniz-Institut für Analytische Wissenschaften-  
ISAS-e.V., Dortmund, Germany
- ThP 129 **Distinct Plasma Molecular Profiles Between Early-onset and Late-onset Colorectal Cancer Patients Revealed by Metabolic and Lipidomic Analyses;** Shiqi Zhang<sup>1</sup>; Rui Xu<sup>1</sup>; Ming Hu<sup>1</sup>; Fouad Choueiry<sup>1</sup>; Ning Jin<sup>1</sup>; Jieli Li<sup>1</sup>; Xiaokui Mo<sup>1</sup>; Jiangjiang Zhu<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH
- ThP 130 **Quantitative Profiling of On-tissue Lipids During Medulloblastoma Metastasis via Aziridination-based Isobaric Mass Tag Labeling and Isomer-resolved Mass Spectrometry Imaging;** Jiaxin Feng<sup>1</sup>; Zilu Huang<sup>2,3</sup>; Dallas Freitas<sup>4</sup>; Tingyuan Yang<sup>4</sup>; Xi Chen<sup>4</sup>; Shuli Tang<sup>4</sup>; Yuhan Yang<sup>5</sup>; Yun Huang<sup>5</sup>; Yuchen Du<sup>2,3</sup>; Xiaonan Li<sup>2,3</sup>; Xin Yan<sup>4</sup>; <sup>1</sup>TAMU, College Station, TX; <sup>2</sup>Ann & Robert H. Lurie Children's Hospital of Chicago, Chicago, IL; <sup>3</sup>Robert H. Lurie Comprehensive Cancer Center, Feinberg School of Medicine, Northwestern University, Chicago, IL; <sup>4</sup>Texas A&M, College Station, TX; <sup>5</sup>Center for Epigenetics & Disease Prevention, Texas A&M Institute of Biosciences and Technology, Houston, TX
- ThP 131 **DESI-MSI Reveals Insights into Metabolic Alterations Associated with Resistance to Immune Checkpoint Inhibitors in Triple Negative Breast Cancer;** Keziah E Liebenberg<sup>1</sup>; Liqun Yu<sup>1</sup>; Meredith L Spradlin<sup>1</sup>; Xiang Zhang<sup>1</sup>; Livia S Eberlin<sup>1</sup>; <sup>1</sup>Baylor College of Medicine, Houston, TX
- ThP 132 **Prostate Cancer Reshapes the Secreted and Extracellular Vesicle Urinary Proteomes;** Amanda Khoo<sup>1</sup>; Meinusha Govindarajan<sup>1</sup>; Zhuyu Qiu<sup>2</sup>; Lydia Y. Liu<sup>1</sup>; Vladimir Ignatchenko<sup>1</sup>; Matthew Waas<sup>1</sup>; Andrew Macklin<sup>1</sup>; Alexander Keszei<sup>1</sup>; Brian P. Main<sup>3</sup>; Lifang Yang<sup>3</sup>; Raymond S. Lance<sup>4</sup>; Michelle R. Downes<sup>5</sup>; O. John Semmes<sup>3</sup>; Danny Vesprini<sup>5</sup>; Stanley Liu<sup>5</sup>; Julius O. Nyalwidhe<sup>3</sup>; Paul C. Boutros<sup>2</sup>; Thomas Kislinger<sup>1</sup>; <sup>1</sup>Princess Margaret Cancer Centre, Toronto, ON; <sup>2</sup>UCLA, Los Angeles, CA; <sup>3</sup>Eastern Virginia Medical School, Norfolk, VA; <sup>4</sup>Spokane Urology, Spokane, WA; <sup>5</sup>Sunnybrook Health Sciences Centre, Toronto, ON
- ThP 133 **A robust metabolic biomarker signature of FASN inhibition;** Dzmitry Mukha<sup>1</sup>; Jena Dessain<sup>1</sup>; Seamus O'Connor<sup>1</sup>; Katherine Pniewski<sup>1</sup>; Fabrizio Bertolazzi<sup>1,2</sup>; Jeet Patel<sup>3</sup>; Mary Mullins<sup>3</sup>; Zachary Schug<sup>1</sup>; <sup>1</sup>The Wistar Institute, Philadelphia, PA; <sup>2</sup>Cellular and Molecular Biology Program, Department of Pharmacy and Biotechnology, University of Bologna, Bologna, Italy; <sup>3</sup>University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA
- ThP 134 **Heterogeneity of drug responses across various lung cancer cell lines with differing genetic backgrounds;** CHUWEI LIN<sup>1</sup>; Devin Schweppe<sup>1</sup>; Katarina Vlajic<sup>1</sup>; Catherine Sniezek<sup>1</sup>; <sup>1</sup>University of Washington - Genome Sciences, Seattle, WA
- ThP 135 **The proteome and post-translational modification landscape of 54 human cancer cell lines - a resource for biomedical studies;** Wenhao Shi<sup>1</sup>; Tianlong He<sup>2</sup>; Nan Wang<sup>3</sup>; Shaojun Tang<sup>2</sup>; Yiyang Zhu<sup>4</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>The Hong Kong University of Science and Technology, Hong Kong, Hong Kong; <sup>3</sup>Fynn Biotechnology, Jinan, China; <sup>4</sup>Tsinghua University, Beijing, China
- ThP 136 **Trapped Ion Mobility Spectrometry (TIMS) enables Deep Coverage of Ras-family members of small GTPases;** Tobias M Maile<sup>1</sup>; Hendry S Cahaya-Healey<sup>1</sup>; Dina J Ghandour<sup>1</sup>; Paul D Schnier<sup>1</sup>; <sup>1</sup>Loxo@Lilly, South San Francisco, CA
- ThP 137 **Proteogenomic biomarkers of recurrence after curative-intent surgery of colorectal liver metastases;** Geoffrey Y.M. Wong<sup>1,2</sup>; Jun Li<sup>2,3</sup>; Matthew J McKay<sup>2,3</sup>; Nazim Bhimani<sup>1</sup>; Connie Diakos<sup>4,5</sup>; Thomas J Hugh<sup>1,5</sup>; Mark P Mollo<sup>2,3</sup>; <sup>1</sup>Department of Upper Gastrointestinal Surgery, Royal North Shore Hospital, Sydney, Australia; <sup>2</sup>Bowel Cancer and Biomarker Laboratory, The University of Sydney, Sydney, Australia; <sup>3</sup>Kolling Institute, Royal North Shore Hospital, Sydney, Australia; <sup>4</sup>Department of Medical Oncology, Royal North Shore Hospital, Sydney, Australia; <sup>5</sup>Northern Clinical School, The University of Sydney, Sydney, Australia
- ThP 138 **Revealing the Phosphorylation and Structural Complexity of Neurofibromin;** Robert A. D'Ippolito<sup>1</sup>; Jennifer Mehalko<sup>1</sup>; Pedro Diaz-Parga<sup>1</sup>; Matthew R. Drew<sup>1</sup>; Scott Eury<sup>1</sup>; Katie Powell<sup>1</sup>; Grace M. Scheidemantle<sup>1</sup>; Vanessa Wall<sup>1</sup>; William Burgan<sup>1</sup>; Dominic Esposito<sup>1</sup>; Frank McCormick<sup>1,2</sup>; Dwight V. Nissley<sup>1</sup>; Caroline J. DeHart<sup>1</sup>; <sup>1</sup>Frederick National Laboratory for Cancer Research, Frederick, MD; <sup>2</sup>Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA
- ThP 139 **Acetylome analysis of aspirin treated AML cell lines using label-free LC-MS/MS reveals potentially cytostatic modifications in cytosolic and mitochondrial proteins;** Luke Higgins<sup>1</sup>; Tommy Shields<sup>1</sup>; Vinothini Rajeeve<sup>1</sup>; Pedro Rodriguez Cutillas<sup>1</sup>; <sup>1</sup>Barts Cancer Institute, Queen Mary University of London, London, United Kingdom
- ThP 140 **Characterizing the role of EED and SUZ12 in the epigenetic reprogramming of MPNST;** Joanna K Lempiainen<sup>1</sup>; Kirill Miachin<sup>1</sup>; Yixuan Axe Xie<sup>1</sup>; Xingyu Liu<sup>1</sup>; Emily Zahn<sup>1</sup>; Kuangying Yang<sup>2</sup>; Angela C Hirbe<sup>2</sup>; Benjamin A Garcia<sup>1</sup>; <sup>1</sup>Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, St. Louis, MO; <sup>2</sup>Division of Oncology, Washington University School of Medicine, St. Louis, MO
- ThP 141 **Cell-type resolved spatial proteogenomics on human FFPE cancer tissue to characterize molecular trajectories in melanoma progression;** Maximilian Zwiebel<sup>1</sup>; Thierry M. Nordmann<sup>1</sup>; Katrin Kerl-French<sup>2</sup>; Rudolf Stadler<sup>3</sup>; Reinhard Dummer<sup>4</sup>; Matthias Mann<sup>1,5</sup>; <sup>1</sup>Department of Proteomics and signal Transduction, Max-Planck-Institute of Biochemistry, Martinsried (near Munich), Germany; <sup>2</sup>Department of Dermatology and Allergy, Ludwig Maximilian University of Munich, Munich, Germany; <sup>3</sup>Department of Dermatopathology, Johannes Wesling Klinikum Minden, Ruhr University Bochum, Minden, Germany; <sup>4</sup>Department of Dermatology, University Hospital Zurich, Zurich, Switzerland; <sup>5</sup>Novo Nordisk Foundation Center for Protein Research (CPR), University of Copenhagen, Copenhagen, Denmark
- ThP 142 **Proteomic Exploration Unveiling the Role of SAP25 in Sin3-Mediated Transcriptional Repression;** Pratik Goswami<sup>1</sup>; Charles A S Banks<sup>2</sup>; Janet Thornton<sup>1</sup>; Bethany Bengs<sup>3</sup>; Mihaela E. Sardi<sup>3,4</sup>; Laurence Florens<sup>2</sup>; Michael P Washburn<sup>1</sup>; <sup>1</sup>Department of Cancer Biology, University of Kansas Medical Center, Kansas City, Kansas 66160; <sup>2</sup>Stowers Institute for Medical Research, Kansas City, Missouri 64110; <sup>3</sup>Department of Biostatistics & Data Science, University of Kansas Medical Center, Kansas City, Kansas; <sup>4</sup>University of Kansas Cancer Center, Kansas City, Kansas
- ThP 143 **Picosecond Infrared Laser Mass Spectrometry enables non-subjective diagnosis of spinal cancers, addressing the high discordance rate in standard of care;** Alexa N Fiorante<sup>1</sup>; Michael Woolman<sup>1</sup>; David Munoz<sup>1</sup>; Gelareh Zadeh<sup>1</sup>; Sunit Das<sup>1</sup>; Howard Ginsberg<sup>1</sup>; Arash Zarrine-Afsar<sup>1</sup>; <sup>1</sup>University of Toronto, Toronto, ON
- ThP 144 **Deep Quantitative Proteomics Identifies Conserved Proteome Alterations in Low and High-Grade Serous Ovarian Cancers;** Jonathan Ogata<sup>1</sup>; Christopher Tarney<sup>1</sup>; Paulette Mhaweche-Fauceglia<sup>1</sup>; Julie Oliver<sup>1</sup>; Tamara Abulez<sup>1</sup>; Brian Hood<sup>1</sup>; Kelly Conrads<sup>1</sup>; Kendal Rosalik<sup>2</sup>; Kwong-Kwok Wong<sup>3</sup>; David Gershenson<sup>3</sup>; Sanghoon Lee<sup>3</sup>; Anil Sood<sup>3</sup>; Kathleen Darcy<sup>1</sup>; Neil Phippen<sup>1</sup>; G. Larry Maxwell<sup>1</sup>; Thomas Conrads<sup>1</sup>; Nicholas W. Bateman<sup>1</sup>; <sup>1</sup>Women's Health Integrated Research Center, Annandale, VA; <sup>2</sup>Department of Gynecologic Surgery and Obstetrics, Madigan Army Medical Center, Joint Base Lewis-McChord, WA; <sup>3</sup>Department of Gynecologic Oncology and Reproductive Medicine, The University of Texas MD Anderson Cancer Center, Houston, TX
- ThP 145 **Understanding Drug Resistance Mechanisms in Lung Cancer: Insights from Proteomic Analysis of ABCB1 Overexpression in A549 Cells;** Geul Bang<sup>1</sup>; Ye Eun Park<sup>2</sup>; Eun Hee Han<sup>2</sup>; Jin Young Kim<sup>2</sup>; <sup>1</sup>Korea Basic Science

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- Institute, Cheongju, South Korea; <sup>2</sup>Korea Basic Science Institute, Cheongju, South Korea
- ThP 146 **Detection of pancreatic cancer cells using aptamers;** Anna Drabik<sup>1</sup>; Joanna Ner-Kluza<sup>2</sup>; Marek Sierzega<sup>2</sup>; <sup>1</sup>AGH University, Krakow, Poland; <sup>2</sup>Department of General, Oncological and Gastrointestinal Surgery, Jagiellonian University Medical College, Krakow, Poland, Krakow, Poland
- ThP 147 **Development of a High-Throughput LC-MS/MS Assay for A-to-I RNA Editing Analysis by ADAR1 in Cancer Drug Discovery;** Timothy He<sup>1</sup>; Jessica MacManus<sup>1</sup>; Lili Guo<sup>1</sup>; Bailin Zhang<sup>1</sup>; <sup>1</sup>Sanofi, Cambridge, MA
- ThP 148 **Characterizing metabolomic heterogeneity in human breast tumour-derived subclonal populations;** Brandon Y. Lieng<sup>1</sup>; William D. Gwynne<sup>1</sup>; Mathula Muhundan<sup>1</sup>; Alexandra J. Denhart<sup>1</sup>; Andrew T. Quaile<sup>1</sup>; Jeremy K. Chan<sup>1</sup>; Nicholas S. Ly<sup>1</sup>; J. Rafael Montenegro-Burke<sup>1</sup>; <sup>1</sup>Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON
- ThP 149 **Analyzing Senolytic Compounds induced Cellular Senescence Response using a Triple Quadrupole Mass Spectrometer;** Evelyn H. Wang<sup>1</sup>; Stephen Kurzyniec<sup>1</sup>; Yoshiyuki Okamura<sup>1</sup>; Yang Yang<sup>2</sup>; Dongwen Lyu<sup>2</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>2</sup>University of Texas Health Science Center at San Antonio, San Antonio, TX
- ThP 150 **Metabolomic Technologies in the bedside diagnosis and treatment of precancerous cervical disease;** Apostolia Galani<sup>1</sup>; Maria Paraskevaidi<sup>1</sup>; Stefania Maneta-Stavrakaki<sup>1</sup>; Daniel Simon<sup>1</sup>; Jinshi Zhao<sup>1</sup>; Burak Temelkuran<sup>1</sup>; Deidre Lyons<sup>1</sup>; Zoltan Takats<sup>1</sup>; Maria Kyrgiou<sup>1</sup>; <sup>1</sup>Imperial College London, London, United Kingdom
- ThP 151 **Decoding the molecular interactions between tumor cells and macrophages with high-throughput proteomic screening of in-vitro co-culture systems for target discovery;** Shreya Ahuja<sup>1</sup>; Becki Dudley<sup>2</sup>; Matthew Glover<sup>1</sup>; Desmond Jones<sup>2</sup>; Sonja Hess<sup>1</sup>; <sup>1</sup>AstraZeneca, Gaithersburg, MD; <sup>2</sup>AstraZeneca, Cambridge, United Kingdom
- ThP 152 **Detections of metabolic activity in human glioblastoma cell lines with U-13C glucose by LC-HR-MS with targeted and untargeted analysis;** Erik Peterson<sup>1</sup>; Liddy McCulla<sup>1</sup>; Li Zhang<sup>1</sup>; Xiaoyi Li<sup>1</sup>; Mack Reynolds<sup>2</sup>; Shivam Panda<sup>1</sup>; Hammad Khan<sup>1</sup>; Harrison Wong<sup>1</sup>; Peter Sajjakulnukit<sup>1</sup>; Costas A Lyssiotis<sup>1</sup>; Daniel Wahl<sup>1</sup>; <sup>1</sup>University of Michigan, Medical School, Ann Arbor, Michigan; <sup>2</sup>University of Michigan, Immunology Program, Ann Arbor, MI
- ThP 153 **Comprehensive Proteogenomic Analysis of Renal Cell Carcinoma Reveals Distinct Molecular Profiles;** Hongyi Liu<sup>1</sup>; Lijun Chen<sup>1</sup>; Yuefan Wang<sup>1</sup>; T. Mamie Lih<sup>1</sup>; Yingwei Hu<sup>1</sup>; Hui Zhang<sup>1</sup>; Clinical Proteomic Tumor Analysis Consortium<sup>2</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD; <sup>2</sup>NIH, Bethesda, MD
- ThP 154 **The proteomic landscape of exhaustion in antigen-specific T cells;** Christian M Beusch<sup>1</sup>; Abdelhameed Dawood<sup>1</sup>; Sarah Welbourn<sup>1</sup>; Ahmet Ozdilek<sup>1</sup>; Mohamed Hakeem<sup>1</sup>; David Gordon<sup>1</sup>; <sup>1</sup>Emory University School of Medicine, Atlanta, GA
- ThP 155 **Cell-type resolved proteomics identifies and quantifies Merkel Cell Polyomavirus proteins directly in Merkel Cell Carcinoma tissue;** Andreas Metousis<sup>1</sup>; Tim Heymann<sup>1</sup>; Lisa Schweizer<sup>1</sup>; Pia-Charlotte Stadler<sup>1,2</sup>; Rudolf Stadler<sup>3</sup>; Thierry M. Nordmann<sup>1</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>Department of Proteomics and Signal Transduction, Max-Planck-Institute of Biochemistry, Martinsried, Germany; <sup>2</sup>Department of Dermatology and Allergology, Ludwig Maximilian University of Munich, Munich, Germany; <sup>3</sup>University Department for Dermatology, Venereology, Allergology and Phlebology, Skin Cancer Center Johannes Wesling Medical Center, Ruhr University Bochum, Minden, Germany
- ThP 156 **Investigating the Role of mSWI-SNF in the Pathogenesis of Malignant Peripheral Nerve Sheath Tumors;** Kirill Miachin<sup>1</sup>; Joanna K Lempiainen<sup>2</sup>; Yixuan Axe Xie<sup>2</sup>; Angela C Hirbe<sup>3</sup>; Benjamin A Garcia<sup>2</sup>; <sup>1</sup>Washington University in Saint Louis, St. Louis, MO; <sup>2</sup>Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, St. Louis, MO; <sup>3</sup>Division of Oncology, Washington University School of Medicine, St. Louis, MO
- ThP 157 **Comparison of LIRADS 5 Image Guided Biopsies From FFPE and Frozen Cores for Radiogenomics and Radioproteomics in Different HCC grades;** Margaret Simonian<sup>1</sup>; David SK Lu<sup>1</sup>; Julian Whitelegge<sup>1</sup>; Whitaker Cohn<sup>1</sup>; Preeti Ahuja<sup>1</sup>; William Hsu<sup>1</sup>; Steven S Raman<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles
- ThP 158 **The distinction of mouse breast cancer by cholesterol profile using ToF-SIMS;** Auraya Manaprasertsak<sup>1</sup>; Per Malmberg<sup>2</sup>; Emma Hammarlund<sup>1</sup>; <sup>1</sup>Lund University, Lund, Sweden; <sup>2</sup>Chalmers University of Technology, Gothenburg, Sweden
- ThP 159 **Unraveling the Mechanism of Cisplatin Resistance in TNBC: Insights from Metabolomic Profiling via Mass Spectrometry Analysis;** Shashwati Parihari<sup>1</sup>; Anvita Pant<sup>2</sup>; Sanjeeva Srivastava<sup>1</sup>; <sup>1</sup>IIT Bombay, Mumbai, India; <sup>2</sup>University of Lausanne, Lausanne, Switzerland
- ThP 160 **Isolation of plasma-derived extracellular vesicles using the Mag-Net method to identify potential protein signatures for diagnosis of pancreatic ductal adenocarcinoma;** Sindiswile Gamelihle Buthelezi<sup>1</sup>; Ireshyn S Govender<sup>1, 2</sup>; Previn Naicker<sup>1</sup>; Andrea Ellero<sup>2, 3</sup>; Stoyan Stoychev<sup>2</sup>; Nnenna Elebo<sup>4</sup>; Jones Omoshoro-Jones<sup>4</sup>; John Devar<sup>4</sup>; Martin Smith<sup>4</sup>; Ekene Emmanuel Nweke<sup>4</sup>; <sup>1</sup>Council for Scientific and Industrial research, Pretoria, South Africa; <sup>2</sup>ReSyn Biosciences, Pretoria, South Africa; <sup>3</sup>University of Pretoria, Pretoria, South Africa; <sup>4</sup>University of the Witwatersrand, Johannesburg, South Africa

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- ThP 161 **Breaking Down Barriers to Point-of-Care Therapeutic Drug Monitoring: Quantitation and Validation of beta-Lactams from Plasma Utilizing Paper Spray Mass Spectrometry;** Hannah Zimmerman-Federle<sup>1</sup>; Nicholas E Manicke<sup>1</sup>; Lindsey Kirkpatrick<sup>1, 2</sup>; <sup>1</sup>IUPUI, Indianapolis, IN; <sup>2</sup>Riley Hospital for Children at Indiana University Health, Indianapolis, Indiana
- ThP 162 **Multidimensional Mass Profiles Increase Confidence in Bacterial Identification When Using Low-Resolution Mass Spectrometers;** Zachary J. Sasiene<sup>1</sup>; Erick S. LeBrun<sup>1</sup>; Nileena Velappan<sup>1</sup>; Austin R. Anderson<sup>1</sup>; Nathan H. Patterson<sup>2</sup>; Martin Dufresne<sup>2</sup>; Melissa A. Farrow<sup>2</sup>; Emilio S. Rivera<sup>1</sup>; Lauren K. Heine<sup>1</sup>; Chi-Yen Tseng<sup>1</sup>; Jessica A. Salgureo<sup>1</sup>; Salvator J. Palmisano<sup>1</sup>; Francisca E. Rodriguez<sup>1</sup>; Tara Harvey<sup>1</sup>; Abigale S. Mikolitis<sup>1</sup>; Kes A. Luchini<sup>1</sup>; Grace M. Thornhill<sup>1</sup>; Brett R. Blackwell<sup>1</sup>; Joshua D. Breidenbach<sup>1</sup>; Phillip M. Mach<sup>1</sup>; Jeremy L. Norris<sup>2</sup>; Richard M. Caprioli<sup>2, 3, 4, 5</sup>; Ethan M. McBride<sup>1</sup>; Trevor G. Glaros<sup>1</sup>; <sup>1</sup>Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>3</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>4</sup>Department of Chemistry, Vanderbilt University, Nashville, TN; <sup>5</sup>Department of Pharmacology, Vanderbilt University, Nashville, TN
- ThP 163 **Proteomics profiling for invasive apocrine breast carcinoma provides subclassification, disease mechanisms and guidance on the administration of chemotherapy;** Yiyang Zhu<sup>1</sup>; Mengping Long<sup>2</sup>; Wenhao Shi<sup>1</sup>; Tianlong He<sup>3</sup>; Taobo Hu<sup>2</sup>; Shaojun Tang<sup>3</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>Peking University, Beijing, China; <sup>3</sup>The Hong Kong University of Science and Technology, Hong Kong, Hong Kong
- ThP 164 **Detection of cocaine derivatives in saliva in 45 seconds: combination of Probe ElectroSpray Ionization (PESI) and quadrupole time-of-flight (QTOF);** Franck SAINT-MARCOUX<sup>1</sup>; Elisa JOUSSELIN<sup>1</sup>; Pauline GRIFFEUILLE<sup>1</sup>; Elies ZARROUK<sup>1</sup>; Souleiman EL BALKHI<sup>1</sup>; <sup>1</sup>University Hospital of Limoges, Limoges, France
- ThP 165 **Paradigm shift in biomarker translation: an innovative and automated pipeline to generate and select clinical-**

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- grade signature peptides during DIA discovery;** Qin Fu<sup>1</sup>; Manasa Vegesna<sup>1</sup>; Niveda Sundararaman<sup>1</sup>; Eugen Damoc<sup>2</sup>; Tabiwang N Arrey<sup>2</sup>; Anna Pashkova<sup>2</sup>; Dalin Li<sup>1</sup>; Jonathan Braun<sup>1</sup>; Dermot P.B. McGovern<sup>1</sup>; Kermit K. Murray<sup>1</sup>; Xuan Yue<sup>2</sup>; Jennifer E. Van Eyk<sup>1</sup>; <sup>1</sup>*Cedars-Sinai Medical Center, Los Angeles, CA*; <sup>2</sup>*Thermo Fisher Scientific, Bremen, Germany*
- ThP 166 **Parallel Reaction Monitoring for Quantitative Detection of Botulinum Neurotoxins in Complex Matrices;** Rose S Atukunda<sup>1</sup>; Karine Bagramyan<sup>1</sup>; Victoria Qiu<sup>1</sup>; Markus Kalkum<sup>1</sup>; <sup>1</sup>*City of Hope, Duarte, CA*
- ThP 167 **Nausea and vomiting in pregnancy is caused by GDF15 produced by the fetus, not the mother;** Amy L George<sup>1</sup>; Emma Cook<sup>2</sup>; Steve D.S Charnock-Jones<sup>2</sup>; Frank Reimann<sup>1</sup>; Fiona M Gribble<sup>1</sup>; Gordon C.S Smith<sup>2</sup>; Stephen O'Rahilly<sup>1</sup>; Richard G Kay<sup>3</sup>; <sup>1</sup>*Wellcome Trust MRC Institute of Metabolic Science, Cambridge, United Kingdom*; <sup>2</sup>*Department of Obstetrics and Gynaecology, University of Cambridge, Cambridge, United Kingdom*; <sup>3</sup>*Wellcome Trust MRC Institute of Metabolic Science, Cambridge, United Kingdom*
- ThP 168 **Selective and Sensitive Analysis of A6-peptide from Mouse Plasma Using LC MS/MS System;** Fatemeh Mousavi<sup>1, 2</sup>; Dan Su<sup>1, 2</sup>; <sup>1</sup>*HD Biosciences, San Diego, CA*; <sup>2</sup>*WuXi AppTec, SAN DIEGO, California*
- ThP 169 **Medical applications of in vivo chemical biopsy probes based on sorbent coated acupuncture needles coupled with LC-MS and direct MS;** Runshan W Jiang<sup>1</sup>; Wei Zhou<sup>1</sup>; Janusz Pawliszyn<sup>1</sup>; <sup>1</sup>*University of Waterloo, Waterloo, ON*
- ThP 170 **Simultaneous determination of three mAbs in human plasma by protein G magnetic beads extraction combined with LC-MS/MS;** Fengmei Hu<sup>1</sup>; Dan Liu<sup>2</sup>; Chao Huang<sup>2</sup>; Xianglong Zhao<sup>2</sup>; Lihai Guo<sup>2</sup>; <sup>1</sup>*Shanghai AB Sciex Analytical Instrument Trading Co.,Ltd., Shanghai, China*; <sup>2</sup>*SCIEX, Shanghai, China*
- ThP 171 **24/7 fully automated therapeutic drug analysis for research projects by LC/MS/MS;** Aureore Jaffuel<sup>1</sup>; Frank Streit<sup>2</sup>; Kohei Yoshikawa<sup>1</sup>; <sup>1</sup>*Shimadzu Corporation, Nakagyo-ku, Japan*; <sup>2</sup>*Department of Clinical Chemistry, University Medical Center Goettingen, Goettingen, Germany*
- ThP 172 **Improvement of system and methods for point-of-care testing of therapeutic drugs with miniature mass spectrometer;** Nan Zhang<sup>1</sup>; Mengyue Xu<sup>1</sup>; Weixu Fan<sup>1</sup>; Jian Zhao<sup>1</sup>; Yuyu Li<sup>1</sup>; Jiexun Bu<sup>1</sup>; Wenpeng Zhang<sup>2</sup>; Zheng Ouyang<sup>2</sup>; <sup>1</sup>*Purspec Technology (Beijing) Ltd., Beijing, China*; <sup>2</sup>*Tsinghua University, Beijing, China*
- ThP 173 **Trace level determination of Polycyclic Aromatic Hydrocarbons in blood plasma using GC-MS/MS;** Santosh Kumar Bhardwaj<sup>1</sup>; Satyendra Pratap Singh Thakur<sup>2</sup>; Mohit Sharma<sup>1</sup>; Jitendra Kelkar<sup>2</sup>; Pratap Rasam<sup>1</sup>; <sup>1</sup>*Shimadzu Analytical (India) Pvt. Ltd., New Delhi, India*; <sup>2</sup>*Shimadzu Analytical (India) Pvt Ltd, New Delhi, India*
- ThP 174 **Using the MSPen Technology for Intraoperative Identification of High-Grade Serous Carcinoma Metastatic Sites During Ovarian Cancer Surgeries;** Charles A. Wolfe<sup>1, 2</sup>; Michael F. Keating<sup>1, 2</sup>; Monica Lin<sup>1</sup>; Ashley E. Montgomery<sup>1</sup>; Barrett C. Lawson<sup>3</sup>; Anil K. Sood<sup>3</sup>; Kelly Rangel<sup>3</sup>; Nicole D. Fleming<sup>3</sup>; Livia S. Eberlin<sup>1</sup>; <sup>1</sup>*Baylor College of Medicine, Houston, TX*; <sup>2</sup>*University of Texas at Austin, Austin, TX*; <sup>3</sup>*MD Anderson Cancer Center, Houston, TX*
- ThP 175 **LC-MS/MS assay for simultaneous quantification of antibiotics in sepsis therapy with efficient purification of clinical samples;** Alina Frieling<sup>1, 2</sup>; Nafissa Agardouh<sup>3</sup>; Malte Bayer<sup>1, 2</sup>; Thilo Bracht<sup>1, 2</sup>; Björn Koos<sup>1</sup>; Hartmuth Nowak<sup>1</sup>; Tim Rahmel<sup>1</sup>; Michael Adamzik<sup>1</sup>; Barbara Sitek<sup>1, 2</sup>; <sup>1</sup>*Clinic for Anesthesiology, Intensive Care and Pain Therapy, University Medical Centre, Knappschaftskrankenhaus Bochum, Bochum, Germany*; <sup>2</sup>*Medical Proteom-Centre, Ruhr-University Bochum, Bochum, Germany*; <sup>3</sup>*Ruhr-University Bochum, Faculty of Biology, Bochum, Germany*
- ThP 176 **SLIMming Down the Workflow: A Novel Approach for Urine Toxicology Analysis;** Miriam Fico<sup>1</sup>; Zongyuan Chen<sup>1</sup>; Alan McKenzie-Coe<sup>1</sup>; Lauren Royer<sup>1</sup>; Joshua K. McBee<sup>1</sup>; Daniel DeBord<sup>1</sup>; Frederick G. Strathmann<sup>1</sup>; <sup>1</sup>*MOBILion Systems, Chadds Ford, PA*
- ThP 177 **A sensitive LC-MS/MS method for relugolix quantification in human plasma and its application to a clinical study;** Sarah Lee<sup>1</sup>; Lan Li<sup>2</sup>; Yuan-Shek Chen<sup>2</sup>; Yulan Chen<sup>1</sup>; <sup>1</sup>*Sumitomo Pharma America, Inc, Marlborough, MA*; <sup>2</sup>*QPS, LLC, Newark, DE*
- ThP 178 **Quantitation of free amino acids in human plasma by Single Quadrupole LC-MS;** TUNA ONCU<sup>1</sup>; Oben Arslan<sup>1</sup>; Ugur Seker<sup>1</sup>; Huseyin Akpinar<sup>1</sup>; <sup>1</sup>*Shimadzu Middle East and Africa FZE Istanbul, Istanbul, Turkey*
- ThP 179 **Pilot study of muscle aging in an older Indian cohort using Metabolomics;** Maroof Athar Hashmi<sup>1</sup>; Arvind Ramanathan<sup>1</sup>; <sup>1</sup>*Institute For Stem Cell Science and Regenerative Medicine, Bengaluru, India*
- ThP 180 **An Automated Sample Preparation Approach for the Determination of Per- and Polyfluoroalkyl Substances (PFAS) from Human Biological Fluids using UHPLC-MS/MS;** Adam Senior<sup>1</sup>; Kyle Bevan<sup>1</sup>; Lee Williams<sup>1</sup>; Geoff Davies<sup>1</sup>; Alan Edgington<sup>1</sup>; Helen Lodder<sup>1</sup>; Russell Parry<sup>1</sup>; Lucy Lund<sup>1</sup>; Zainab Khan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Dan Menasco<sup>1</sup>; <sup>1</sup>*Biotage GB Limited, Cardiff, United Kingdom*
- ThP 181 **A 2D Microfluidic Paper-Based Analytical Device for Diagnosis of Canine Visceral Leishmaniasis in Developing Countries;** Hianka J. C. De Carvalho<sup>1, 2</sup>; Ayesha Seth<sup>2</sup>; Ruth M. Speidel<sup>2</sup>; Maria A. Miglino<sup>1</sup>; Abraham K. Badu-Tawiah<sup>2</sup>; <sup>1</sup>*Universidade de Sao Paulo, Sao Paulo, Brazil*; <sup>2</sup>*The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio*
- ThP 182 **Rapid Methicillin-Resistant Staphylococcus aureus Screening Software Based on MALDI-TOF MS and Machine Learning: A Multi-Center Assessment of Clinical Performance;** Jong-Min Park; *Hallym University, Chuncheon, South Korea*
- ThP 183 **Result and Interpretation Discrepancies In-Between Urine Drug Confirmatory Screen performed by UPLC-ESI-MS/MS Methods: Importance of Method Development and Validation;** Amanda Toupin<sup>1</sup>; Candace Fowler<sup>2</sup>; Benoît Denhez<sup>3</sup>; Pierre-Luc Mallet<sup>3</sup>; <sup>1</sup>*Université de Sherbrooke, Sherbrooke, QC*; <sup>2</sup>*Eastern Health, St. John's, NL*; <sup>3</sup>*CIUSSSE-CHUS, Sherbrooke*
- ThP 184 **EXPANDING STEROID PROFILING BY UHPLC-MS/MS ANALYSIS OF ENDOGENOUS HORMONES AND PHASE II METABOLITES: INVESTIGATION OF CIRCADIAN VARIATIONS;** Federico Ponzetto<sup>1</sup>; Mirko Parasiliti-Caprino<sup>1</sup>; Laura Leoni<sup>2</sup>; Lorenzo Campioni<sup>1</sup>; Lorenzo Marinelli<sup>1</sup>; Fabio Settanni<sup>3</sup>; Antonello Nonnato<sup>3</sup>; Ezio Ghigo<sup>1</sup>; Roberta Giordano<sup>4</sup>; Giulio Mengozzi<sup>2, 3</sup>; <sup>1</sup>*Endocrinology, Diabetology and Metabolism, Department of Medical Sciences, University of Turin, Turin, Italy*; <sup>2</sup>*Clinical Biochemistry Laboratory, Department of Medical Sciences, University of Turin, Turin, Italy*; <sup>3</sup>*Clinical Biochemistry Laboratory, City of Health and Science University Hospital, Turin, Turin, Italy*; <sup>4</sup>*Department of Clinical and Biological Sciences, University of Turin, Turin, Italy*
- ThP 185 **Empower the Quantitation of Amino Acids and Acylcarnitine for Inborn Error of Metabolism using Flow Injection – Orbitrap Mass Spectrometer;** Jingshu Guo<sup>1</sup>; Yvonne Song<sup>1</sup>; Kerry Hassell<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*
- ThP 186 **LC-MS/MS Screening Tests for Drug Abuse: Three Years of Experience at A Tertiary Hospital in Korea;** Ju Hyeon Lee<sup>1</sup>; Ayeong Bak<sup>1</sup>; Jongsun Joo<sup>1</sup>; Jikyo Lee<sup>1</sup>; Sang Hoon Song<sup>1</sup>; <sup>1</sup>*Seoul National University Hospital, Seoul, South Korea*
- ThP 187 **Integrating Genomics, Proteomics, and Metabolomics Data within the NIH Multi-Omics for Health and Disease Consortium;** Cassandra G Kempf<sup>1, 2</sup>; Ethan Stancliffe<sup>3</sup>; Michaela Schwaiger-Haber<sup>2</sup>; Dhanalakshmi S Anbukumar<sup>1</sup>; Leah P Shriver<sup>1, 2, 4</sup>; Gary J. Patti<sup>1, 2, 4</sup>; <sup>1</sup>*Department of Chemistry, Washington University in St. Louis, Saint Louis, MO*; <sup>2</sup>*Center for Proteomics, Metabolomics and Isotope Tracing, Washington University in St. Louis, St. Louis, MO*;

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<sup>3</sup>Panome Bio, St Louis, MO; <sup>4</sup>Department of Medicine, Washington University in St. Louis, Saint Louis, MO

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- ThP 189 **Quantitative Amine to Acid Chemical Crosslinking: Towards the Completion of the Conformationome of Alpha-Synuclein and its Proteoforms**; Ashlyn N Dollar<sup>1</sup>; Ian K Webb<sup>1</sup>; <sup>1</sup>Indiana University Indianapolis, Indianapolis, IN
- ThP 190 **A covalent labeling-mass spectrometry based method for high-throughput screening of amyloid inhibitors**; Kanitin Khamnong<sup>1</sup>; Richard Vachet<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Massachusetts Amherst, Amherst, MA
- ThP 191 **Characterization of Protein Structure by Top-Down Cleavable Crosslinking**; Erika Renbarger<sup>1</sup>; Ian K Webb<sup>1</sup>; <sup>1</sup>Indiana University Indianapolis, Indianapolis, IN
- ThP 192 **Covalent Labeling Mass Spectrometry of a Membrane Protein on Live Cells Using a Label Enrichment Strategy**; Ina De La Fuente<sup>1</sup>; Elise Blackstock<sup>1</sup>; Richard Vachet<sup>1</sup>; <sup>1</sup>University of Massachusetts Amherst, Amherst, MA
- ThP 193 **LC separation optimization for XL-MS Analysis**; Yi He<sup>1</sup>; Erum Raja<sup>2</sup>; Leigh Foster<sup>2</sup>; Max Ruwolt<sup>3</sup>; Anthony Ciancone<sup>4</sup>; Fan Liu<sup>3</sup>; Francis O'Reilly<sup>4</sup>; Ryan Bomgarden<sup>2</sup>; Rosa Viner<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Rockford, Illinois; <sup>3</sup>Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; <sup>4</sup>NIH, Frederick, MD
- ThP 194 **Automated Hydroxyl Radical Protein Footprinting in a 96-Well Format**; Jiana Duan<sup>1</sup>; Zhi Cheng<sup>1</sup>; Emily Hart<sup>1</sup>; Casey Y. O'Connell<sup>1</sup>; Armando Santos-Landa<sup>1</sup>; Calyx Liu<sup>1</sup>; Robert Egan<sup>1</sup>; Joshua S Sharp<sup>1, 2</sup>; Scot Weinberger<sup>1</sup>; <sup>1</sup>GenNext Technologies, Half Moon Bay, CA; <sup>2</sup>UNIVERSITY OF Mississippi, Oxford, MS
- ThP 195 **Fast and accurate disulfide bridge detection**; Richard Scheltema<sup>1</sup>; Søren Heissel<sup>2</sup>; Yi He<sup>3</sup>; Andris Jankevics<sup>1</sup>; Henrik Molina<sup>2</sup>; Rosa Viner<sup>3</sup>; <sup>1</sup>Liverpool University, Liverpool, United Kingdom; <sup>2</sup>Proteomics Resource Center, The Rockefeller University, New York, New York; <sup>3</sup>ThermoFisher Scientific, San Jose, CA
- ThP 196 **Studying the Tau and Low-Density Lipoprotein Receptor-Related Protein 1 complex interface through Diethylpyrocarbonate - Based Covalent Labeling Mass Spectrometry**; Vanessa L. Stahl<sup>1</sup>; Trisha W. Brady<sup>2</sup>; Zachary J. Kirsch<sup>2</sup>; Jennifer N. Rauch<sup>1,3</sup>; Richard W. Vachet<sup>1, 2</sup>; <sup>1</sup>Molecular & Cellular Biology Program, University of Massachusetts Amherst, Amherst, MA; <sup>2</sup>Department of Chemistry, University of Massachusetts Amherst, Amherst, MA; <sup>3</sup>Department of Biochemistry & Molecular Biology, University of Massachusetts Amherst, Amherst, MA
- ThP 197 **Comparing an Epitope Identified from a Crystal Structure with In-solution Mass Spectrometry-based Techniques Including HRP and XL-MS**; Zhi Cheng<sup>1</sup>; Emily Chea<sup>1</sup>; Rosa Viner<sup>2</sup>; Rodney G. King<sup>3</sup>; Guang Yang<sup>3</sup>; R. Glenn King<sup>3</sup>; Todd J. Green<sup>3</sup>; John T. Killian, Jr.<sup>3</sup>; Peter E. Prevelige<sup>3</sup>; Frances E. Lund<sup>3</sup>; Scot Weinberger<sup>1</sup>; <sup>1</sup>GenNext Technologies, Half Moon Bay, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>University of Alabama Birmingham, Birmingham, Alabama
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- ThP 199 **Cross-linking coupled to mass spectrometry (XLMS) for structural elucidation of antimicrobial peptide complexes: example of PGLa/Mag2**; Emilie Hirschler<sup>1</sup>; Elise Glattard<sup>2</sup>; Yannis-Nicolas François<sup>1</sup>; Burkhard Bechinger<sup>2</sup>; Emmanuelle Leize-Wagner<sup>1</sup>; Noelle Potier<sup>1</sup>; <sup>1</sup>Laboratoire de spectrométrie de masse des interactions et des systèmes, UMR 7140, University of Strasbourg, Strasbourg, France; <sup>2</sup>Laboratoire de biophysique des membranes et RMN, UMR 7177, University of Strasbourg, Strasbourg, France
- ThP 200 **Identification of acidic amino acid side chains in proteins by selective chemical labeling and tandem mass spectrometry**; Akash Talukder<sup>1</sup>; Ashima Mehta<sup>1</sup>; Aisosa Omere<sup>1</sup>; Sepideh Khaki Firooz<sup>1</sup>; Joseph Anthony Buonomo<sup>1</sup>; Saiful M Chowdhury<sup>1</sup>; <sup>1</sup>University of Texas at Arlington, Arlington, TX
- ThP 201 **Constructing a FPOP Spectral Library for Accurate Identification of Modified Amino Acids**; Haolin Luo<sup>1</sup>; Nuno Bandeira<sup>2,3,4</sup>; Lisa M. Jones<sup>1</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA; <sup>2</sup>Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; <sup>3</sup>Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; <sup>4</sup>Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA
- ThP 202 **Discovering Crosslinks with Parallel Reaction Monitoring**; Lindsey D. Ulmer<sup>1</sup>; Lucas Narisawa<sup>1</sup>; Christopher N. Woods<sup>2</sup>; Natalie L. Stone<sup>2</sup>; Maria K. Janowska<sup>2</sup>; Rachel E. Klevit<sup>2</sup>; Matthew F. Bush<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Washington, Seattle, WA; <sup>2</sup>Department of Biochemistry, University of Washington, Seattle, WA
- ThP 203 **Conventional cell fixation improves performance of in situ crosslinking mass spectrometry while preserving cellular ultrastructure.**; Andrew RM Michael<sup>1</sup>; Bruno C Amaral<sup>1</sup>; David C Schriemer<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, AB
- ThP 204 **In-Cell Structural Determination of NFκB Inhibition by IκBα**; Luis Oliva<sup>1</sup>; Lisa M. Jones<sup>1</sup>; Elizabeth A. Komives<sup>1</sup>; <sup>1</sup>University of California San Diego, La Jolla, CA
- ThP 205 **Automatized SCX fractionation combined with 4-CV Gas Phase fractionation boosts crosslinks identifications in both in-vitro and proteome-wide XL-MS workflows**; Hugo Gizardin-Fredon<sup>1, 2</sup>; Alexandre GEFFROY<sup>1, 2</sup>; Fabrice BERTILE<sup>1, 2</sup>; Sarah Cianferani<sup>1, 2</sup>; <sup>1</sup>Laboratoire de Spectrométrie de Masse BioOrganique, IPHC UMR 7178, Université de Strasbourg, CNRS, Strasbourg, France; <sup>2</sup>Infrastructure Nationale de Protéomique ProFI – FR2048, Strasbourg, France
- ThP 206 **Trapped-ion mobility spectrometry with PASEF for identification and quantification of protein-RNA crosslinks**; Sergey Moshkovskii<sup>1</sup>; Olexandr Dybkov<sup>1</sup>; Timo Sachsenberg<sup>2, 3</sup>; Ralf Pflanz<sup>1</sup>; Monika Raabe<sup>1</sup>; Oliver Kohlbacher<sup>2, 3, 4</sup>; Henning Urlaub<sup>1, 5</sup>; <sup>1</sup>Bioanalytical Mass Spectrometry Group, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; <sup>2</sup>Applied Bioinformatics, Dept. of Computer Science, University of Tübingen, Tübingen, Germany; <sup>3</sup>Institute for Bioinformatics and Medical Informatics, University of Tübingen, Tübingen, Germany; <sup>4</sup>Institute for Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany; <sup>5</sup>Bioanalytics, Department of Clinical Chemistry, University Medical Center Göttingen, Göttingen, Germany
- ThP 207 **Inter-species click-linking: an improved strategy to estimate false discovery rates for protein-protein interactions detected by XL-MS**; Alex Crowder<sup>1</sup>; Bruno C

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- ThP 208 **Navigating IgG-antiCH1 Binding Landscapes with Integrated Protein Footprinting Techniques to Assist Streamlined Purification Development**; Pengyi Zhao<sup>1</sup>; Yu Shi<sup>1</sup>; <sup>1</sup>AstraZeneca, Gaithersburg, MD
- ThP 209 **Alzheimer's disease related amyloid-beta misfolding studied by gas-phase carbene footprinting mass spectrometry**; Paul Martino; Houghton University, Houghton, NY
- ThP 210 **Probing the structural surfaceome of cancer cell models to identify tumor-specific protein conformations**; Audrey A Kishishita<sup>1</sup>; Abhilash Barpanda<sup>1</sup>; Arthur Zalevsky<sup>1</sup>; Deeptharup Biswas<sup>2</sup>; Ayushi Verma<sup>2</sup>; Sanjyot Vinayak Shenoy<sup>2</sup>; Michael R Hoopmann<sup>3</sup>; Clinton Yu<sup>4</sup>; Fenglong Jiao<sup>4</sup>; Lan Huang<sup>4</sup>; Robert L Moritz<sup>3</sup>; Andrej Sali<sup>1</sup>; Sanjeeva Srivastava<sup>2</sup>; Arun P Wiita<sup>1</sup>; <sup>1</sup>UCSF, San Francisco, CA; <sup>2</sup>IIT Bombay, Mumbai, India; <sup>3</sup>Institute for Systems Biology, Seattle, Washington; <sup>4</sup>UCI, IRVINE, CA
- ThP 211 **Assessing a tyrosine-reactive functionality for covalent labeling and crosslinking applications: Introducing novel reagents for protein structural and interaction studies**; Saiful Chowdhury<sup>1</sup>; Adway Ouseph Zacharias<sup>2</sup>; Sharel Cornelius<sup>2</sup>; <sup>1</sup>University of Texas at Arlington, Arlington, TX; <sup>2</sup>University of Texas at Arlington, Arlington, TX
- ThP 212 **A Photocatalytic Proximity-Labeling Platform Utilizing Commercially Available Reagents for Micro-mapping the Dynamics of Surface Receptor Protein Complexes During Target Engagement**; David H. Perlman<sup>1</sup>; Ritchie Ly<sup>2</sup>; Clementina Strozek<sup>2</sup>; Paolo Cifani<sup>3</sup>; Michelle Sao<sup>2</sup>; Travis Hartman<sup>2</sup>; Justin R Cross<sup>2</sup>; <sup>1</sup>Health Outlook, New York, NY; <sup>2</sup>Memorial Sloan Kettering Cancer Center, New York, NY; <sup>3</sup>Cold Spring Harbor Laboratory, Cold Spring Harbor, NY
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- ThP 214 **Novel mass spectrometry-based immuno-immobilization functional assay for the structure-activity relationship determination of modulators for a transmembrane sterol isomerase**; Reza Nemati Josheghani<sup>1</sup>; Ronghai Cheng<sup>1</sup>; Meiyi Zhang<sup>2</sup>; Daniel Tekverk<sup>1</sup>; Howard Jones<sup>1</sup>; Martin Himmelbauer<sup>1</sup>; <sup>1</sup>Biogen, Cambridge, MA; <sup>2</sup>Texas A&M, College Station, TX
- ThP 215 **The battle for sensitivity: practical strategies for boosting signal-to-noise ratio in LC-MS/MS quantitative analysis supporting drug discovery**; Yue-Ting Wang; AbbVie, North Chicago, IL
- ThP 216 **A Validated HILIC-HRMS Method for Quantitative Analysis of Synthetic Oligonucleotides**; Md Rabiul Islam<sup>1</sup>; A M Abdullah<sup>1</sup>; Cynthia Sommers<sup>1</sup>; Jason Rodriguez<sup>1</sup>; Deyi Zhang<sup>2</sup>; Darby Kozak<sup>2</sup>; Kui Yang<sup>1</sup>; <sup>1</sup>U.S. Food and Drug Administration, St. Louis, MO; <sup>2</sup>U.S. Food and Drug Administration, Silver Spring, MD
- ThP 217 **High-Throughput Mass Spectrometry Based Screening Approach for Quantitative Protein-Ligand Affinity Measurements in Pooled Compound Libraries**; Craig B Gutierrez<sup>1</sup>; Neal Liddle<sup>1</sup>; Feizhi Ding<sup>1</sup>; Nomaan Rezayee<sup>1</sup>; Fred Manby<sup>1</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>Iambic Therapeutics, San Diego, CA
- ThP 218 **Quantitative Analysis of Dithiothreitol (DTT) and Oxidized DTT in Three Acidified Cell Culture Media by LC/MS/MS**; Wen Lin<sup>1</sup>; Timothy White<sup>1</sup>; Erika Stark<sup>1</sup>; <sup>1</sup>Charles River Laboratories, Worcester, MA
- ThP 219 **Systematic identification and validation of degrader drug targets by deep proteomic screening and high-sensitivity ubiquitinomics**; Uli Ohmayer<sup>1</sup>; Martin Steger<sup>1</sup>; Björn Schwalb<sup>1</sup>; Gisele Nishiguchi<sup>2</sup>; Kevin McGowan<sup>2</sup>; Jutta Fritz<sup>1</sup>; Vadim Demichev<sup>3</sup>; Zoran Rankovic<sup>2</sup>; Henrik Daub<sup>1</sup>; <sup>1</sup>NEOsphere Biotechnologies GmbH, Planegg, Germany; <sup>2</sup>Department of Chemical Biology & Therapeutics, St. Jude Children's Research Hospital, Memphis, TN; <sup>3</sup>Charité, Universitätsmedizin Berlin, Berlin, Germany
- ThP 220 **Discovery of a novel, gut microbial small molecule that improves immunotherapy response in mice with humanized microbiomes**; Jasmine Chong<sup>1</sup>; Cuong Nguyen<sup>1</sup>; Greg Fedewa<sup>1</sup>; Leslie Sedgeman<sup>1</sup>; Antonio Carmona<sup>1</sup>; Miriam Velez<sup>1</sup>; Nathan Wan<sup>1</sup>; Yan Yang<sup>1</sup>; Sarkis Mazmanian<sup>2</sup>; Bryan Yoo<sup>1</sup>; <sup>1</sup>Nuanced Health, Los Angeles, CA; <sup>2</sup>California Institute of Technology, Pasadena, CA
- ThP 221 **Characterization of antibody coverage for anti-HCP ELISA by nanoLC-MS/MS**; Jia Guo<sup>1</sup>; Yiran Liang<sup>1</sup>; Regina Kufer<sup>2</sup>; Stefanie Wohlrab<sup>2</sup>; Midori Greenwood-Goodwin<sup>1</sup>; Feng Yang<sup>1</sup>; <sup>1</sup>Genentech, South San Francisco, CA; <sup>2</sup>Roche Diagnostics GmbH, Penzberg, Germany
- ThP 222 **LC-MS/MS quantification of total IgG of intravenous immunoglobulin (IVIg) in mouse plasma**; Dominic Bounkhoun<sup>1</sup>; Jose Trinidad<sup>1</sup>; Hsin Chen<sup>1</sup>; Weixuan Chen<sup>1</sup>; <sup>1</sup>Johnson and Johnson, San Diego, CA
- ThP 223 **Detecting protein-protein interaction directly using crosslinking and high-mass MALDI mass spectrometry for SARS-CoV-2 drug discovery**; Congrui Tan<sup>1</sup>; Yuye Zhou<sup>1,2</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland; <sup>2</sup>KTH Royal Institute of Technology, Stockholm, Sweden
- ThP 224 **Label-free native MS-based screening of PROTACs and molecular glues**; Edvaldo V. S. Maciel<sup>1</sup>; Christian Meyners<sup>1</sup>; Felix Hausch<sup>1</sup>; Tanja Habeck<sup>1</sup>; Frederik Lermyte<sup>1</sup>; <sup>1</sup>Technical University of Darmstadt, Clemens-Schöpf-Institute for Organic Chemistry and Biochemistry, Darmstadt, Germany
- ThP 225 **Development and Validation of a Sensitive LC-APCI-MS/MS Method to Quantify a Poorly-ionized Drug, Pocapavir, in C57BL/6 Mouse Plasma**; Renmeng Liu<sup>1</sup>; Ashley Davie<sup>1</sup>; Elaine To<sup>1</sup>; Yurong Lai<sup>1</sup>; <sup>1</sup>Gilead Sciences Inc., Foster City, CA
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- ThP 227 **iBA (intelligent BioAnalysis): Pioneering the Future of Bioanalysis**; Romina Schnegotzki<sup>1</sup>; Svenja Mayer-Wrangowski<sup>1</sup>; Siegfried Wild<sup>1</sup>; Anne-Michaela Kuebler<sup>1</sup>; Wolfgang Joerg<sup>2</sup>; Juergen Weber<sup>2</sup>; Christian Spaeth<sup>2</sup>; Christoph Disch<sup>2</sup>; Andreas H. Luippold<sup>1</sup>; <sup>1</sup>Drug Discovery Sciences, DDS, Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach, Germany; <sup>2</sup>Lab Equipment Solutions, LES, Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach, Germany
- ThP 228 **A High Throughput and Robust Assay for Quantifying a Bi-Specific Peptide Drug Conjugate (CRCPAC90387) in Human Plasma Using HPLC-MS/MS**; Limin Chu<sup>1</sup>; Robert Huang<sup>2</sup>; Hongfang (Andy) Xue<sup>1</sup>; Mo Xu<sup>2</sup>; Laixin Wang<sup>1</sup>; Guitao Wang<sup>2</sup>; Yuehui Ma<sup>1</sup>; Fan Pan<sup>2</sup>; Aining Li<sup>2</sup>; Aihua Liu<sup>1</sup>; <sup>1</sup>Resoliant (Formerly Alliance Pharma), Malvern, PA; <sup>2</sup>Coherent Biopharma, Hefei, China
- ThP 229 **Development of a high-throughput tissue sample processing approach for CETSA MS**; Mariel Grace R Mendoza<sup>1</sup>; Matthew Mazur<sup>1</sup>; Christopher Novotny<sup>2</sup>; Anu Sebini<sup>2</sup>; Weixun Wang<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., West Point, PA; <sup>2</sup>Merck, South San Francisco, CA
- ThP 230 **Parallel Global Metabolite Profiling and Characterization of Potential Drug Metabolites in Three-dimensional Hepatospheroids**; Darshak Gadara<sup>1, 2, 3</sup>; Songjie Chen<sup>4</sup>; Leah P. Shriver<sup>1, 2, 3</sup>; Thuy Tran<sup>4</sup>; Oscar Ekpenyong<sup>4</sup>; Dan Rock<sup>4</sup>; Gary J. Patti<sup>1, 2, 3</sup>; <sup>1</sup>Department of Chemistry, Washington University in St. Louis, Saint Louis, MO; <sup>2</sup>Center for Proteomics, Metabolomics and Isotope Tracing, Washington University in St. Louis, Saint Louis, MO; <sup>3</sup>Department of Medicine, Washington University in St. Louis, Saint Louis, MO; <sup>4</sup>Department of Pharmacokinetics, Dynamics, Metabolism and Bioanalytics, Merck & Co., Inc., South San Francisco, CA

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- ThP 231 **A Proteomics-Based Platform for High-Throughput Screening of Kinase Inhibitors;** Ravi Tharakan<sup>1</sup>; Yanyan Qu<sup>1</sup>; Yuhong Fang<sup>1</sup>; Patrick J. Morris<sup>1</sup>; Michele Ceribelli<sup>1</sup>; Craig J Thomas<sup>1</sup>; Christopher A LeClair<sup>1</sup>; Dingyin Tao<sup>1</sup>; <sup>1</sup>National Center for Advancing Translational Sciences, NIH, Rockville, MD
- ThP 232 **Role of density functional theory in explaining MS/MS fragmentation mechanism of biologically active substituted urea derivative quizartinib;** Sudam S Mane<sup>1</sup>; David V Dearden<sup>1</sup>; <sup>1</sup>Brigham Young University, Provo, UT
- ThP 233 **Auranofin targets UBA1 and enhances activity by facilitating ubiquitin transthioesterification to E2 ubiquitin conjugating enzymes;** Dingyin Tao<sup>1</sup>; Yanyan Qu<sup>1</sup>; Christopher A LeClair<sup>1</sup>; Shengyun Fang<sup>2</sup>; <sup>1</sup>National Center for Advancing Translational Sciences, NIH, Rockville, MD; <sup>2</sup>University of Maryland, Baltimore, Baltimore, MD
- ThP 234 **A simple, direct and sensitive LC-MS/MS method for the determination of cationic lipid in human liver microsomes;** Jiao Zhang<sup>1</sup>; Dan Li<sup>1</sup>; Yangzhen Zheng<sup>1</sup>; Juanjuan Zhu<sup>1</sup>; Jinlian Lu<sup>1</sup>; Zhiyu Li<sup>1</sup>; Lili Xing<sup>1</sup>; Yi Tao<sup>1</sup>; Liang Shen<sup>1</sup>; <sup>1</sup>WuXi AppTec, Shanghai, China
- ThP 235 **Deploying an Ultra-Sensitive, High-Throughput, Integrated Microflow LC-MS/MS System to Support in vitro PK/PD Assessment;** Brendon Kapinos<sup>1</sup>; Jamie Tourville<sup>1</sup>; Qianying Yuan<sup>1</sup>; Ashley Bertrand<sup>1</sup>; Mitchell Laughlin<sup>1</sup>; Tom Schroeter<sup>1</sup>; Steve Ainley<sup>2</sup>; Wayne Lootsma<sup>2</sup>; <sup>1</sup>Pfizer, Groton, CT; <sup>2</sup>Sound Analytics, Deep River, CT
- ThP 236 **Isotyping and quantitation of anti-AAV antibody in human serum by immunoprecipitation coupled to liquid chromatography and mass spectrometry;** Xiaoxiao Huang<sup>1</sup>; Yuetian Yan<sup>1</sup>; Sven Moller-Tank<sup>1</sup>; Shunhai Wang<sup>1</sup>; Ning Li<sup>1</sup>; <sup>1</sup>Regeneron Pharmaceuticals, Tarrytown, NY
- ThP 237 **Development of a Validated LC-MS/MS Method for the Quantification of Psilocin in Mouse Plasma: Addressing a Major Interference;** Amir Khajavinia<sup>1</sup>; Deborah Michel<sup>1</sup>; Udoka C Ezeaka<sup>1</sup>; Randy W Purves<sup>1,2</sup>; Robert B Laprarie<sup>1</sup>; Anas El-Aneed<sup>1</sup>; <sup>1</sup>University of Saskatchewan, Saskatoon, SK; <sup>2</sup>Canadian Food Inspection Agency, Saskatoon, SK
- EPIGENETIC MODIFICATIONS**  
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- ThP 238 **Defining histone proteoforms in prenucleosome complexes and nucleosomes in centromeric and global chromatin by Top-Down Mass Spectrometry;** Alexander S Lee<sup>1,2</sup>; Che-Fan Huang<sup>1</sup>; Daniel R. Foltz<sup>2</sup>; Neil L. Kelleher<sup>1,2</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Northwestern University Feinberg School of Medicine, Chicago, IL
- ThP 239 **Utilization of Immunoprecipitation to Assess H3.3K36M Oncohistone Proteoforms and Post-Translational Modifications for Quantitative Top-Down Mass Spectrometry;** Alyssa Paparella<sup>1</sup>; Karl F. Poncha<sup>1</sup>; Cheryl L. Walker<sup>1</sup>; Nicolas L. Young<sup>1</sup>; <sup>1</sup>Baylor College of Medicine, Houston, TX
- ThP 240 **Systematic Characterization of Recombinant and Endogenous Chlamydomonas reinhardtii SET-Domain Methyltransferases by Biochemical and Mass Spectrometric Approaches;** Michael Hayes<sup>1</sup>; James J Pesavento<sup>1</sup>; <sup>1</sup>Saint Mary's College, Moraga, CA
- ThP 241 **Identification of histone lysine acetoacetylation as a dynamic post-translational modification regulated by HBO1;** Yan Gao<sup>1</sup>; Xinlei Sheng<sup>2</sup>; Doudou Tan<sup>3</sup>; Sunjoo Kim<sup>1</sup>; He Huang<sup>3</sup>; Yingming Zhao<sup>2</sup>; Sangkyu Lee<sup>4</sup>; <sup>1</sup>College of Pharmacy, Kyungpook National University, Daegu, South Korea; <sup>2</sup>The University of Chicago, Chicago, IL; <sup>3</sup>Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China; <sup>4</sup>School of Pharmacy, Sungkyunkwan University, Suwon, South Korea
- ThP 242 **An optimized workflow for monitoring the canonical histone ubiquitination marks H2AK119ub and H2BK120ub by LC-MS/MS;** Peder J. Lund<sup>1</sup>; Mariana Lopes<sup>1</sup>; Benjamin A. Garcia<sup>2</sup>; <sup>1</sup>Department of Nutrition, Case Western Reserve University, School of Medicine, Cleveland, OH; <sup>2</sup>Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, St. Louis, MO
- ThP 243 **Top down proteomics reveals a proteoform-truncation mechanism that supersedes the DNA damage and apoptotic response;** Faith M. Joseph<sup>1</sup>; Matthew V. Holt<sup>1</sup>; Nicolas L. Young<sup>2</sup>; <sup>1</sup>Baylor College of Medicine, Houston, Texas; <sup>2</sup>Baylor College of Medicine, Houston, TX
- ThP 244 **Scoring Post-translational Modification Crosstalk from Histone Proteoform Data;** Karl F. Poncha<sup>1</sup>; Alyssa T. Paparella<sup>2</sup>; Nicolas L. Young<sup>1,2,3</sup>; <sup>1</sup>Verna and Marrs McLean Department of Biochemistry and Molecular Pharmacology, Baylor College of Medicine, Houston, TX; <sup>2</sup>Center for Precision Environmental Health, Baylor College of Medicine, Houston, TX; <sup>3</sup>Department of Molecular and Cellular Biology, Baylor College of Medicine, Houston, TX
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- ThP 245 **Quantification and Identification of Arsenic Species in Freshwater Fish Using HPLC-ICPMS/ESIMS;** Chester Lau<sup>1</sup>; Xiufen Lu<sup>2</sup>; Tetiana Davydiuk<sup>1</sup>; Jennifer A. Graydon<sup>3</sup>; Megan Reichert<sup>3</sup>; Ruth Mitchell<sup>3</sup>; X. Chris Le<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, University of Alberta, Edmonton, AB; <sup>2</sup>Department of Laboratory Medicine and Pathology, University of Alberta, Edmonton, AB; <sup>3</sup>Alberta Health, Health Protection Branch, Edmonton, AB
- ThP 246 **Direct injection screening method for Per-and-polyfluoroalkyl substances in drinking water using a prototype benchtop multi-reflecting Time-of-flight;** Hania Khoury-Hollins<sup>1</sup>; Stuart Adams<sup>1</sup>; Jayne Kirk<sup>1</sup>; Richard Lock<sup>1</sup>; Lance Nicolaysen<sup>2</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Waters, Milford, MA
- ThP 247 **Orbitrap isotopic ratio mass spectrometry of methylated stearic acid and its application to vegetable butter source discrimination;** Gabriel Franco Dos Santos<sup>1</sup>; Alexis Gilbert<sup>2</sup>; Giovanni B. Bevilacqua<sup>1</sup>; Hugo G. Machado<sup>1</sup>; Maxime Julien<sup>3</sup>; Gesiane S. Lima<sup>1</sup>; Nerilson M. Lima<sup>1</sup>; Júlio C. O. Ribeiro<sup>1</sup>; Alexandre A. Ferreira<sup>4</sup>; Ygor S. Rocha<sup>4</sup>; Boniek G. Vaz<sup>1</sup>; <sup>1</sup>Federal University of Goiás, Goiânia, Brazil; <sup>2</sup>Tokyo Institute of Technology, Tokyo, Japan; <sup>3</sup>Université de Nantes, CNRS, Nantes, France; <sup>4</sup>PETROBRAS, Rio de Janeiro, Brazil
- ThP 248 **Measuring per- and polyfluoroalkyl substances in baby formula powder: A quantitative LC-MS/MS approach;** Matthew Noestheden<sup>1, 2</sup>; Karl Oetjen<sup>3</sup>; Simon Roberts<sup>3</sup>; <sup>1</sup>SCIEX, Concord, ON; <sup>2</sup>University of British Columbia, Vancouver, BC; <sup>3</sup>Sciex, Framingham, MA
- ThP 249 **Confirming veterinary drug residues in problematic samples using a rapid FAIMS-based strategy with existing diagnostic LC-MS methods;** Randall W Purves<sup>1</sup>; Michael W. Belford<sup>2</sup>; Bryn O. Shurmer<sup>1</sup>; Jana Kinar<sup>1</sup>; <sup>1</sup>Canadian Food Inspection Agency, Saskatoon, SK; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 250 **Development of a high-resolution MRM quantitative method for pesticides in apple, honey, olive oil, orange and tomato food matrices;** Alan Barnes<sup>1</sup>; Raquel Leonardo<sup>2</sup>; Emily G Armitage<sup>1</sup>; Jonathan McGeehan<sup>3</sup>; Steve Williams<sup>2</sup>; Neil J Loftus<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Manchester, United Kingdom; <sup>2</sup>SGS Cambridge Limited, Cambridge, United Kingdom; <sup>3</sup>Shimadzu UK Limited, Milton Keynes, United Kingdom
- ThP 251 **Quantitation of Zearalenone and Deoxynivalenol in Zea Mays using LC-MS;** Valeria Zerda-Pinto<sup>1</sup>; Charlette Hasty<sup>2</sup>; Mary-Margaret B Benware<sup>1</sup>; Tyson Lobb<sup>1</sup>; Ifeoluwa P Osikoya<sup>1</sup>; Fatima Romo<sup>1</sup>; Olufunke M Ayegbidun<sup>1</sup>; Logan M Stenger<sup>3</sup>; John A Juvik<sup>3</sup>; Laura A Chatham<sup>3</sup>; Tiffany M Jamann<sup>3</sup>; Anthony J Studer<sup>3</sup>; Martin O Bohn<sup>3</sup>; Carolyn Butts-Willmsmeyer<sup>1</sup>; Kevin Tucker<sup>1</sup>; <sup>1</sup>Southern Illinois University Edwardsville, Edwardsville, IL; <sup>2</sup>Southern Illinois University Carbondale, Carbondale, IL; <sup>3</sup>University of Illinois Urbana-Champaign, Champaign, IL
- ThP 252 **Determination of Ergot Alkaloids in Cereal-based Food using LC-MS/MS;** Weili Xiong<sup>1</sup>; Christian Talavera<sup>1</sup>; <sup>1</sup>U.S. Food and Drug Administration, College Park, MD
- ThP 253 **An Integrated GC-MS/MS and LC-MS/MS Workflow for Quantitative Analysis of Pesticides with Cross-**



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- confirmation using a **Single Chromatography Data System Software**; [Ed George](#)<sup>1</sup>; Julie Moriceau<sup>2</sup>; Delphine Thomas<sup>3</sup>; Jean-François Garnier<sup>2</sup>; Richard Fussell<sup>4</sup>; Toby Astill<sup>1</sup>; <sup>1</sup>ThermoFisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific GmbH, Bremen, Germany; <sup>4</sup>Thermo Fisher Scientific, Hemel Hempstead, United Kingdom
- ThP 254 **LC-MS/MS-based dilute-and-shoot approach for the quantitation of more than 800 pesticides and mycotoxins: challenges and solutions**; [Jianru Stahl-Zeng](#)<sup>1</sup>; Hassan El Khallabi<sup>2</sup>; Jack Steed<sup>3</sup>; Said El Ouali<sup>4</sup>; Ian Moore<sup>5</sup>; <sup>1</sup>SCIEX, Darmstadt, Germany; <sup>2</sup>Normec Groen Agro Control, Delfgauw, Netherlands; <sup>3</sup>SCIEX UK, Macclesfield, United Kingdom; <sup>4</sup>SCIEX, Darmstadt, Germany; <sup>5</sup>SCIEX, Concord, ON
- ThP 255 **Utilizing hydrogen carrier gas for sensitive analysis of pesticides in food using gas chromatography mass spectrometry**; [Adam Ladak](#)<sup>1</sup>; Paul Silcock<sup>2</sup>; Xin Zheng<sup>3</sup>; Jason Cole<sup>3</sup>; Amit Gujar<sup>3</sup>; Daniel Kutscher<sup>4</sup>; Nicholas Warner<sup>4</sup>; <sup>1</sup>Thermo Scientific, Macclesfield, United Kingdom; <sup>2</sup>Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; <sup>3</sup>Thermo Fisher Scientific, Bannockburn, IL; <sup>4</sup>Thermo Fisher Scientific, Bremen, Germany
- ThP 256 **A Dietary Glycan Encyclopedia of Food: Unveiling Molecular Structures via LC-MS for Precision Nutrition Initiatives**; [Shawn Ehlers-Cheang](#)<sup>1</sup>; Christopher Suarez<sup>1</sup>; Jules A Larke<sup>2, 3</sup>; Jiani Jiang<sup>1</sup>; Cheng-Yu Charlie Weng<sup>1</sup>; Aaron D Stacy<sup>1</sup>; Danielle G Lemay<sup>2, 3</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of California, Davis, Davis, CA; <sup>2</sup>Department of Food Science and Technology, University of California, Davis, Davis, CA; <sup>3</sup>Western Human Nutrition Research Center, USDA Agricultural Research Service, Davis, CA
- ThP 257 **Determination of 31 Per- and Poly-fluoroalkyl Substances in Food Packaging with APGC-MS/MS and UPLC-MS/MS**; [Chia-Yang Chen](#)<sup>1, 2</sup>; I-Chieh Hu<sup>2</sup>; <sup>1</sup>Institute of Food Safety and Health, National Taiwan University, Taipei City, Taiwan; <sup>2</sup>Institute of Environmental and Occupational Health Sciences, National Taiwan University, Taipei City, Taiwan
- ThP 258 **Method Validation for Determining 513 Pesticide Residues in Cucumber Using LCMS-8060NX and 308 Residues by GCMS-TQ8040NX**; [Anant Lohar](#)<sup>1</sup>; Rakan Saad Abdullah Alajmi<sup>2</sup>; Hatim Zaid Ali Alhazmi<sup>2</sup>; Sarah Awwadh Sultan Alotaibi<sup>2</sup>; Jayachandran Namasivayam<sup>3</sup>; Shailesh Damale<sup>1</sup>; Jessin Mathai<sup>1</sup>; <sup>1</sup>Shimadzu Middle East and Africa FZE, Dubai, United Arab Emirates; <sup>2</sup>Saudi Food and Drug Authority, Riyadh, Saudi Arabia; <sup>3</sup>AnalyticaOne Group, Doha, Qatar
- ThP 259 **Comparison of sample preparation for determination of mycotoxins in cannabis and cannabis derived products using LC-FLD and LC-MS/MS**; [Giorgia Greco](#)<sup>1</sup>; Juliane Kramer<sup>1</sup>; Susanne Huhmann<sup>1</sup>; <sup>1</sup>KNAUER, Berlin, Germany
- ThP 260 **Ultra-fast multiresidues accurate mass screening strategy**; [Olivier Chevallier](#)<sup>1</sup>; Cate Simmermaker<sup>1</sup>; Kai Chen<sup>1</sup>; Chris Klein<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- ThP 261 **New model to optimize triple quadrupole mass spectrometer performance for fast SRM methods**; [Michael Ugarov](#)<sup>1</sup>; Harald Oser<sup>1</sup>; Hans Schweingruber<sup>1</sup>; Neloni Wijeratne<sup>1</sup>; Agnès Le Corre<sup>2</sup>; Claudia Martins<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Courtaboeuf, France
- ThP 262 **Sulfite Quantification in Foods and Beverages Using Single Quadrupole LC-MS**; Saho Yoshioka<sup>1</sup>; Nozomi Maeshima<sup>1</sup>; [Dominika Gruszecka](#)<sup>2</sup>; Landon Wiest<sup>2</sup>; Ryo Yamaguchi<sup>1</sup>; Manami Kobayashi<sup>1</sup>; <sup>1</sup>SHIMADZU Corporation, Kawasaki, Japan; <sup>2</sup>Shimadzu Scientific Instruments, Columbia, MD
- ThP 263 **Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Fish Fillet with LC-MS/MS**; [Kota Ishioka](#)<sup>1</sup>; Nozomi Maeshima<sup>1</sup>; Toshiya Matsubara<sup>2</sup>; Manami Kobayashi<sup>1</sup>; <sup>1</sup>SHIMADZU Corporation, Kawasaki, Japan; <sup>2</sup>Shimadzu Scientific Instruments, Columbia, MD
- ThP 264 **Simultaneous Analysis of Pesticides in Food With GC-MS/MS Using Hydrogen Carrier Gas**; [Nozomi Maeshima](#)<sup>1</sup>; Kyoko Yamada<sup>1</sup>; Yoshihiro Saito<sup>1</sup>; Dominika Gruszecka<sup>2</sup>; Alan Owens<sup>2</sup>; Manami Kobayashi<sup>1</sup>; <sup>1</sup>SHIMADZU Corporation, Kawasaki, Japan; <sup>2</sup>Shimadzu Scientific Instruments, Columbia, MD
- ThP 265 **Determination of mycotoxins in dry feed for small animals**; [Laudicéia Alves De Oliveira](#)<sup>1</sup>; Marcelo Viana De Moraes<sup>2</sup>; Edivaldo Domingues Velini<sup>2, 3</sup>; Ichiro Hirano<sup>1</sup>; Marcos Albieri Pudenzi<sup>1</sup>; <sup>1</sup>Shimadzu do Brasil, Barueri, Brazil; <sup>2</sup>Bioativa, Botucatu, Brazil; <sup>3</sup>Universidade Estadual Paulista - UNESP, Botucatu, Brazil
- ThP 266 **Investigating Per- and Poly-Fluoroalkyl Substances (PFAS) Interferences in Food Matrices with High-Resolution Mass Spectrometry**; [Brian Ng](#)<sup>1</sup>; Christine M Fisher<sup>1</sup>; Susan Genualdi<sup>1</sup>; Wendy Young<sup>1</sup>; Elsie Peparh<sup>1</sup>; Lowri De Jager<sup>1</sup>; <sup>1</sup>U.S. Food and Drug Administration, College Park, MD
- ThP 267 **Reliable determination of anionic polar pesticides in fruits and vegetables by using LC-MS/MS**; [Samruddha Chavan](#)<sup>1</sup>; Nitin Shukla<sup>1</sup>; Nitish Ramchandra Suryawanshi<sup>1</sup>; Nilesh Patil<sup>1</sup>; Ramesh Manigiri<sup>1</sup>; Shraddha Kadam<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; Pratap Rasam<sup>1</sup>; <sup>1</sup>Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- ThP 268 **Application of a Novel Automated Sample Preparation Platform for the Determination of Acrylamide in Instant Coffee and Analysis using UPLC-MS/MS**; Russell Parry<sup>1</sup>; Helen Lodder<sup>1</sup>; Alan Edgington<sup>1</sup>; Lee Williams<sup>1</sup>; Charlotte Hayes<sup>1</sup>; Geoff Davies<sup>1</sup>; Adam Senior<sup>1</sup>; Lucy Lund<sup>1</sup>; Zainab Khan<sup>1</sup>; Claire Desbrow<sup>1</sup>; [Dan Menasco](#)<sup>1</sup>; <sup>1</sup>Biotage GB Limited, Cardiff, United Kingdom
- ThP 269 **Simultaneous Determination of Alternaria Toxins, Ergot Alkaloid Epimers, and Other Major Mycotoxins in Various Food Matrices by LC-MS/MS**; [Diego A Lopez](#)<sup>1</sup>; Shun-Hsin Liang<sup>1</sup>; Justin Steimling<sup>1</sup>; <sup>1</sup>Restek Corporation, Bellefonte, PA
- ThP 270 **Mass spectrometric characterization of natural protein sweeteners for evaluation as substitutes for artificial sweeteners**; [SEPIDEH KHAKI FIROOZ](#)<sup>1</sup>; Saiful M Chowdhury<sup>2</sup>; <sup>1</sup>University of Texas at Arlington (UTA), Arlington, TX; <sup>2</sup>University of Texas at Arlington, Arlington, TX
- ThP 271 **How to deal with sweet matrix? – a method for LC-MS/MS analysis of antibiotics in honey, regardless of its kind**; [Julia Mironenka](#)<sup>1</sup>; Rafal Szewczyk<sup>1, 2</sup>; Katarzyna Krupczyńska-Stopa<sup>1, 2</sup>; Maciej Stopa<sup>1, 2</sup>; <sup>1</sup>LabExperts sp. z o.o. NIP:5833181181, Gdansk, Poland; <sup>2</sup>Bioanalytic sp z o.o., Gdańsk, Poland
- ThP 272 **Development of a QuEChERS-based UPLC-MS/MS for the Simultaneous Determination of Neonicotinoids, Parabens, and Bisphenols in Vegetables and Biscuits**; [Hsin-Chang Chen](#)<sup>1</sup>; Zou-Xiao Huang<sup>2</sup>; Jung-Wei Chang<sup>3</sup>; Po-Chin Huang<sup>4, 5, 6</sup>; <sup>1</sup>Department of Chemistry, Tunghai University, Taichung City, Taiwan; <sup>2</sup>Institute of Food Safety and Health, National Taiwan University, Taipei City, Taiwan; <sup>3</sup>Institute of Environmental and Occupational Health Sciences, School of Medicine, National Yang Ming Chiao Tung University, Taipei, Taiwan; <sup>4</sup>National Institute of Environmental Health Sciences, National Health Research Institutes, Miaoli, Taiwan; <sup>5</sup>Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; <sup>6</sup>Department of Medical Research, China Medical University Hospital, China Medical University, Taichung City, Taiwan
- ThP 273 **Advanced Solid-Phase Extraction Methods for Rapid Pesticide Residue Analysis Compatible with Both GC-MS and LC-MS/MS, Utilizing QuEChERS Extraction**; [Takumi Kunieda](#)<sup>1</sup>; Manabu Takayanagi<sup>1</sup>; Shigenori Ota<sup>1</sup>; <sup>1</sup>GL Sciences Inc., Saitama, Japan

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- ThP 274 **Rapid detection and classification of near-neighbor fentanyl variants by 2D MS/MS and machine learning**; Dalton Snyder<sup>1</sup>; Megan Guetzloff<sup>1</sup>; Jane Likens<sup>1</sup>; Anthony

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- Eshleman<sup>1</sup>; Andrew Houvenagle<sup>1</sup>; Kevin Rosenbaum<sup>1</sup>; Austin Stieglitz<sup>1</sup>; Brandon Reese<sup>1</sup>; Mitch Wells<sup>1</sup>; <sup>1</sup>*Teledyne FLIR, West Lafayette, IN*
- ThP 275 **Characterization of oligomeric 2-butanone peroxide species and the associated gas-phase and solution-phase rearrangement products by electrospray ionization**; Ryan M Bain<sup>1</sup>; John Stutzman<sup>2</sup>; Julie Pannuto<sup>1</sup>; Meghan Kane<sup>1</sup>; <sup>1</sup>*Bureau of Alcohol, Tobacco, Firearms and Explosives, Beltsville, MD*; <sup>2</sup>*Dow Inc, Midland, MI*
- ThP 276 **Identification of Isobaric Methyl-Substituted Fentanyl Analogs using a Transportable Linear Ion Trap Mass Spectrometer**; Alleigh N. Couch<sup>1</sup>; J. Tyler Davidson<sup>1</sup>; <sup>1</sup>*Department of Forensic Science, Sam Houston State University, Huntsville, TX*
- ThP 277 **Enhanced Genetically Variant Peptide Profiling from Human Hair Using Keratinase and Trypsin**; Zheng Zhang<sup>1</sup>; William E. Wallace<sup>1</sup>; Guanghui Wang<sup>1</sup>; Meghan C. Burke<sup>1</sup>; Yi Liu<sup>1</sup>; Stephen E. Stein<sup>1</sup>; <sup>1</sup>*NIST, Gaithersburg, MD*
- ThP 278 **Analysis of Explosives using Laser Diode Thermal Desorption (LDTD) coupled to a Orbitrap mass spectrometer**; Amanda Wrison<sup>1</sup>; Gina M. Guerrero<sup>1</sup>; Eshwar Jagerdeo<sup>1</sup>; <sup>1</sup>*FBI, Quantico, VA*
- ThP 279 **Detecting human contaminant genetically variant peptides from unknown sources**; Fanny Chu<sup>1</sup>; Andy Lin<sup>1</sup>; Daniel Lewis<sup>1</sup>; Sarah Jenson<sup>1</sup>; Robert W. Seymour<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*
- ThP 280 **Illicit Drug Desorption and Chemical Profiling of Fingerprints using SICRIT Ion Source: A Rapid Analysis Approach**; Ciara Conway<sup>1, 2</sup>; Markus Weber<sup>1, 2</sup>; Allison Ferranti<sup>2</sup>; Jan-Christoph Wolf<sup>2</sup>; Christoph Haisch<sup>1</sup>; <sup>1</sup>*Technical University of Munich, Freising, Germany*; <sup>2</sup>*Plasmion GmbH, Augsburg, Germany*
- ThP 281 **Simultaneous screening of nearly 300 synthetic cannabinoids and metabolites in blood and urine samples using an LC-QTOF system**; Jiahong Xiang<sup>1</sup>; Yan Shi<sup>2</sup>; Yukun Chen<sup>3</sup>; Zong Yang<sup>3</sup>; Bingjie Liu<sup>3</sup>; Lihai Guo<sup>3</sup>; <sup>1</sup>*College of Forensic Medicine, Hebei Medical University, Shijiazhuang, China*; <sup>2</sup>*Department of Forensic Toxicology, Academy of Forensic Science, Shanghai Key Laboratory of Forensic Medicine, Shanghai Forensic Science Platform, Key Laboratory of Forensic Sciences, Ministry of Justice, Shanghai, China*; <sup>3</sup>*SCIEX Asia Pacific Application Support Center, Shanghai, China*
- ThP 282 **Automated solid-phase extraction with gas chromatography-mass spectrometry for high-throughput analysis and application of narcotic drugs in human urine**; Chohee Jeong<sup>1</sup>; Hamin Choi<sup>1</sup>; Sang Beom Han<sup>1</sup>; <sup>1</sup>*Dept of Pharmaceutical Analysis, College of Pharmacy, Chung-Ang University, Seoul, South Korea*
- ThP 283 **Cannabinoids Isomeric Profiling in Seized Materials by LC-ESI(±)LTQ MS**; Wanderson Romão<sup>1, 2</sup>; João Victor M. De Almeida<sup>3</sup>; Nathália S. Conceição<sup>2, 3</sup>; Marcos Valério V. Lyrio<sup>3</sup>; Nayara A. dos Santos<sup>2, 3</sup>; Rafael S. Ortiz<sup>2, 4</sup>; <sup>1</sup>*Federal Institute of Espirito Santo, Brazil, Vitória, Brazil*; <sup>2</sup>*National Institute of Forensic Science and Technology, INCT, Porto Alegre, Brazil*; <sup>3</sup>*Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espirito Santo, Vitória, Brazil*; <sup>4</sup>*Technical-Scientific Sector, Regional Superintendence of the Federal Police Department in Rio Grande do Sul, Brazil, Porto Alegre, Brazil*
- ThP 284 **Simultaneous detection of cocaine and its metabolites in urine samples by direct analysis using Cellulose Fiber Spray Ionization Mass Spectrometry**; Nayara Araujo Dos Santos<sup>1, 2</sup>; Nathália dos Santos Conceição<sup>1, 2</sup>; Sara Joaquina I. Dionisio<sup>1</sup>; Emmily Travassos Alves<sup>1</sup>; Bruna Carneiro Pires<sup>2</sup>; Wanderson Romão<sup>1, 2, 3</sup>; <sup>1</sup>*Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espirito Santo, Vitória, Brazil*; <sup>2</sup>*National Institute of Forensic Science and Technology, INCT, Porto Alegre, Brazil*; <sup>3</sup>*Federal Institute of Espirito Santo, Brazil, Vila Velha, Brazil*
- ThP 285 **Application of a novel screening workflow for the detection of illicit and medicinal drugs in human hair**; Emily G Armitage<sup>1</sup>; Thomas Brema<sup>2</sup>; Christopher Bowen<sup>3</sup>; Alan Barnes<sup>1</sup>; Rohan Steel<sup>4</sup>; Neil J Loftus<sup>1</sup>; <sup>1</sup>*Shimadzu Corporation, Manchester, United Kingdom*; <sup>2</sup>*Shimadzu Deutschland GmbH, Duisburg, Germany*; <sup>3</sup>*Shimadzu Scientific Instruments, Melbourne, Australia*; <sup>4</sup>*Biological Research Unit, Racing Analytical Services Limited, Flemington, Australia*
- ThP 286 **Forensic Applications of a Validation and Implementation Package for Rapid GC-MS Analysis of Seized Drugs and Ignitable Liquids**; Briana A. Capistran<sup>1</sup>; Elizabeth L. Robinson<sup>1</sup>; Edward Sisco<sup>1</sup>; <sup>1</sup>*National Institute of Standards and Technology, Gaithersburg, MD*
- ThP 287 **Untargeted High Resolution Mass Spectrometry and Molecular Networking for Forensic Toxicology Screening of Drugs of Abuse**; Maia Bates<sup>1</sup>; Abby Helm<sup>1</sup>; Heather M Barkholtz<sup>1</sup>; <sup>1</sup>*University of Wisconsin-Madison, Madison, WI*
- ThP 288 **Development of a screening method for 93 fentanyl analogues in teabag using LC-MS/MS with serially coupled columns**; Jiyu Kim<sup>1</sup>; Sang Beom Han<sup>1</sup>; <sup>1</sup>*Dept of Pharmaceutical Analysis, College of Pharmacy, Chung-Ang University, Seoul, South Korea*
- ThP 289 **A New Workflow for Fast Elucidation of Drug Metabolites for Screening – A Story of Microsomes and Microchips**; Annette Zschesche<sup>1</sup>; Birgit Schneider<sup>2</sup>; Ilona Nordhorn<sup>2</sup>; Carsten Baessmann<sup>2</sup>; Laura M. Huppertz<sup>1</sup>; Jürgen Kempf<sup>1</sup>; <sup>1</sup>*Institute of Forensic Medicine, Medical Center - University of Freiburg, Freiburg, Germany*; <sup>2</sup>*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*
- ThP 290 **Analyzing the chemical footprints of toxic and hazardous compounds in dust particles in real-time using Single-Particle Mass Spectrometry**; Heinrich Ruser<sup>1</sup>; Johannes Passig<sup>2, 3</sup>; Sven Ehlert<sup>4</sup>; Haseeb Hakim<sup>2</sup>; Marco Schmidt<sup>2</sup>; Aleksandrs Kalamasnikovs<sup>2</sup>; Michael Pütz<sup>5</sup>; Petra Hehet<sup>5</sup>; Martin Seipenbusch<sup>6</sup>; Karsten Wegner<sup>6</sup>; Andreas Walte<sup>4</sup>; Ralf Zimmermann<sup>2, 3</sup>; <sup>1</sup>*University of the Bundeswehr Munich, Neubiberg, Germany*; <sup>2</sup>*University of Rostock, Rostock, Germany*; <sup>3</sup>*Joint Mass Spectrometry Centre, Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Munich, Munich, Germany*; <sup>4</sup>*Photonion GmbH, Schwerin, Germany*; <sup>5</sup>*Federal Criminal Police Office, Forensic Science Institute, Wiesbaden, Germany*; <sup>6</sup>*ParteQ GmbH, Malsch, Germany*
- ThP 291 **Sensitive UHPLC-MS/MS and enantioselective SFC-MS method for determination of pharmacokinetic profiles of methoxphenidine and its metabolite in biological matrices**; Natalie Paškanová<sup>1</sup>; Magdalena Vagnerova<sup>2</sup>; Bronislav Jurásek<sup>1</sup>; Martin Kuchar<sup>1</sup>; Michal Kohout<sup>3</sup>; <sup>1</sup>*Department of Chemistry of Natural Compound and Forensic Laboratory of Biologically Active Substances, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic*; <sup>2</sup>*Department of Analytical Chemistry, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic*; <sup>3</sup>*Department of Organic Chemistry, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic*
- ThP 292 **T-ReXing Synthetic Cannabinoid Receptor Agonists – Unveiling Metabolites Suitable for Urine Screening via UHPLC-timsTOF-MS and MetaboScope**; Annette Zschesche<sup>1</sup>; Birgit Schneider<sup>2</sup>; Ilona Nordhorn<sup>2</sup>; Carsten Baessmann<sup>2</sup>; Jürgen Kempf<sup>1</sup>; Laura M. Huppertz<sup>1</sup>; <sup>1</sup>*Institute of Forensic Medicine, Medical Center - University of Freiburg, Freiburg, Germany*; <sup>2</sup>*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*
- ThP 293 **Rapid analysis of explosives on surfaces using new LDTD Ion Source in less than 9 seconds per sample**; Serge Auger<sup>1</sup>; Jonathan Rochon<sup>1</sup>; Mégane Moreau<sup>1</sup>; Sarah Demers<sup>1</sup>; Jean Lacoursière<sup>1</sup>; Pierre Picard<sup>1</sup>; <sup>1</sup>*Phytronix Technologies, Quebec, QC*
- ThP 294 **Rapid screening and quantitation of forensically-relevant samples using LC-timsTOF**; William J Feeney<sup>1</sup>; Edward Sisco<sup>1</sup>; <sup>1</sup>*National Institute of Standards and Technology, Gaithersburg, MD*

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- ThP 295 **Noninvasive Soil Vapor Probe (SVP) and LIDAR Assisted TO-15 GC/MS Quantitative VOCs Analyses for Searching in Clandestine Burial Investigations;** Brian A Eckenrode<sup>1</sup>; Timothy Nelligan<sup>2</sup>; Steve Hoyt<sup>3</sup>; <sup>1</sup>George Mason University, Aldie, VA; <sup>2</sup>Katahdin Environmental Corp, San Clemente, CA; <sup>3</sup>Environmental Analytical Service, Inc., San Luis Obispo, CA
- ThP 296 **Equine Doping Control Analysis with Negative Ion Electropray High-Resolution Mass Spectrometry;** Youwen You<sup>1,2</sup>; Jaclyn R. Missanelli<sup>1,2</sup>; Rachel M. Proctor<sup>1,2</sup>; Mary A. Robinson<sup>1,2</sup>; <sup>1</sup>University of Pennsylvania School of Veterinary Medicine, Pennsylvania, PA; <sup>2</sup>Pennsylvania Equine Toxicology & Research Laboratory, West Chester, Pennsylvania
- ThP 297 **Detection of xylazine-laced fentanyl using a novel acoustic ejection HRMS;** Aaron Stella<sup>1</sup>; Jacob Watson McCabe<sup>2</sup>; Anuja Bhalkikar<sup>2</sup>; Babu Purkayastha<sup>2</sup>; <sup>1</sup>SCIEX, Framingham, MA; <sup>2</sup>Sciex, Framingham, MA
- ThP 298 **A handheld Van de Graaff generator for combined sampling and ionization in fieldable mass spectrometry of trace drug residues;** Kenyon Evans-Nguyen<sup>1</sup>; Paige K Hunt<sup>1</sup>; Kimberly Edmunds<sup>1</sup>; Mackenzie Sampson<sup>2</sup>; La'Nyah Nance<sup>1</sup>; Julia X Morelli<sup>1</sup>; <sup>1</sup>The University of Tampa, Tampa, FL; <sup>2</sup>University of South Florida, Tampa, FL
- ThP 299 **Analysis of trace metals content of illicit cocaine for source attribution using ICP-MS;** Edward Bentil<sup>1</sup>; Brian A Eckenrode<sup>2</sup>; <sup>1</sup>George Mason University, Manassas, VA; <sup>2</sup>George Mason University, Manassas, Virginia
- ThP 300 **Inclusive Sample Cleanup Approaches for Broad-spectrum Drugs of Abuse Whole Blood Analysis;** Kyle Dukes<sup>1</sup>; Yuan Li<sup>1</sup>; Lee Williams<sup>2</sup>; Esraa EboJasser<sup>1</sup>; <sup>1</sup>Biotage, Charlotte, NC; <sup>2</sup>Biotage GB Limited, Cardiff, United Kingdom
- ThP 301 **High precision isotope ratio Orbitrap-MS, a novel tool for vanillin authentication;** Nils Johannes Kuhlbusch<sup>1,2</sup>; Issaku E. Kohl<sup>2</sup>; Dieter Juchelka<sup>2</sup>; Heiko Hayden<sup>1</sup>; David Psomiadis<sup>3</sup>; Balázs Horváth<sup>3</sup>; Andreas Hilkert<sup>2</sup>; <sup>1</sup>University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; <sup>2</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; <sup>3</sup>Imprint Analytics GmbH, Neutal, Austria
- ThP 302 **How to improve the precision of analysis - semi-automated sample preparation for psychoactive compounds quantification in human plasma;** Maciej Stopa<sup>1</sup>; Julia Mironenka<sup>2</sup>; Rafal Szewczyk<sup>1,2</sup>; Anna Lenartowicz<sup>2</sup>; Adrian Soboń<sup>1,3</sup>; Katarzyna Krupczyńska-Stopa<sup>1</sup>; <sup>1</sup>Bioanalytic Sp. z o.o., Gdansk, Poland; <sup>2</sup>LabExperts sp z o.o., Gdańsk, Poland; <sup>3</sup>LabExperts sp. z o.o. NIP:5833181181, Gdansk, Poland
- ThP 303 **Evaluating the Use of nLC on Several Mass Spectrometers for the Full Scan Forensic Analysis of Xylazine Illicit Drug Mixtures;** Mehdi Moini<sup>1</sup>; Brian A Eckenrode<sup>2</sup>; Edward Bentil<sup>1</sup>; <sup>1</sup>Picolytics, McLean, VA; <sup>2</sup>George Mason University, Manassas, Virginia

### FUNDAMENTALS: ION SPECTROSCOPY 304-308

- ThP 304 **Infrared Multiple Photon Dissociation Spectroscopic Evidence for Challenges to Density Functional Theory: Metal Carbenes and Cesiated Glycine;** Peter B. Armentrout<sup>1</sup>; Joost Bakker<sup>2</sup>; Ryan P. Steele<sup>1</sup>; Brandon C. Stevenson<sup>1</sup>; Jonathan Martens<sup>2</sup>; Giel Berden<sup>2</sup>; Jos Oomens<sup>2</sup>; <sup>1</sup>University of Utah, Salt Lake City, UT; <sup>2</sup>Radboud University, Nijmegen, Netherlands
- ThP 305 **Probing Microsolvation-Induced Alteration of the Structure of Deprotonated Leucine Enkephalin via Helium Nanodroplet Isolation Infrared Action Spectroscopy;** Madeline Schultz<sup>1</sup>; Katja Ober<sup>2</sup>; América Y Torres-Boy<sup>2</sup>; Maleesha T Fernando<sup>1</sup>; Miyuru M Wellalage<sup>1</sup>; Nwanne D Banor<sup>1</sup>; Martín I Taccone<sup>2</sup>; Gert von Helden<sup>2</sup>; Daniel A Thomas<sup>1</sup>; <sup>1</sup>University of Rhode Island Chemistry Department, Kingston, Rhode Island; <sup>2</sup>Fritz Haber Institute of the Max Planck Society, Berlin, Germany
- ThP 306 **New Instrumentation for Infrared Action Spectroscopy of Trapped Ions from Ambient Temperature to 400 mK;**

Madeline Schultz<sup>1</sup>; Neil A Ellis<sup>1</sup>; Nwanne D Banor<sup>1</sup>; Maleesha T Fernando<sup>1</sup>; Miyuru M Wellalage<sup>1</sup>; Daniel A. Thomas<sup>1</sup>; <sup>1</sup>University of Rhode Island Chemistry Department, Kingston, Rhode Island

- ThP 307 **2-cyanoindenyl Radical Anion Isomers: Predicted Negative Ion Photoelectron Spectra and Isomer Specific Thermochemistry;** Dushmantha Namal Koku Hannadige Abeysooriya<sup>1</sup>; Nolan J White<sup>1</sup>; Wilson K Gichuhi<sup>1</sup>; <sup>1</sup>Tennessee Tech University, Cookeville, TN
- ThP 308 **Gas-Phase Coordination of Phosphine-Chalcogenides to the Uranyl Cation;** Christopher Zarzana<sup>1</sup>; JungSoo Kim<sup>1</sup>; Brittany D. M. Hodges<sup>1</sup>; Madeline Martelles<sup>2</sup>; Jonathan Martens<sup>3</sup>; Giel Berden<sup>3</sup>; Cristian Celis Barros<sup>4</sup>; Thomas Albrecht-Schoenart<sup>2</sup>; <sup>1</sup>Idaho National Laboratory, Idaho Falls, ID; <sup>2</sup>Colorado School of Mines, Golden, CO; <sup>3</sup>Radboud University, Nijmegen, Netherlands; <sup>4</sup>Oak Ridge National Laboratory, Oak Ridge, TN

### FUNDAMENTALS: IONIC CLUSTERS, NANOMATERIALS, AND CATALYSIS 309-311

- ThP 309 **Structural Investigation of Deep Eutectic Solvents by Infrared Action Spectroscopy in Helium Nanodroplets and Condensed-Phase Analysis;** Miyuru M Wellalage<sup>1</sup>; Maleesha T Fernando<sup>1</sup>; Emily M Molino<sup>1</sup>; América Y Torres-Boy<sup>2</sup>; Katja Ober<sup>2</sup>; Madeline Schultz<sup>1</sup>; Nwanne D Banor<sup>1</sup>; Neil A Ellis<sup>1</sup>; Gert von Helden<sup>2</sup>; Daniel A Thomas<sup>1</sup>; <sup>1</sup>University of Rhode Island, Kingston, RI; <sup>2</sup>Fritz Haber Institute of the Max Planck Society, Berlin, Germany
- ThP 310 **Electrospray Ionization Mass Spectrometry Reveals the Biofunctionalization of a Silver Lipolate Nanocluster with Amino Acids!** Joseph Goldenberg<sup>1</sup>; David Black<sup>2</sup>; Marcos Alvarez<sup>1</sup>; Mozammel Hoque<sup>3</sup>; Robert Whetten<sup>3</sup>; <sup>1</sup>Los Angeles Mission College, Sylmar, CA; <sup>2</sup>University of Texas at San Antonio, San Antonio, TX; <sup>3</sup>Northern Arizona University, Flagstaff, AZ
- ThP 311 **Gas-phase chemistry of the photo-reduced [Mo6I13]2-cluster species;** Aikaterini Tsirkou<sup>1</sup>; Richard A. J. O'Hair<sup>2</sup>; Karine Costuas<sup>3</sup>; Fabien Grasset<sup>3</sup>; Yann Molard<sup>3</sup>; Stéphane Cordier<sup>3</sup>; Luke MacAleese<sup>1</sup>; <sup>1</sup>Institut Lumière Matière, UMR5306 CNRS & UCBL, Lyon, France; <sup>2</sup>University of Melbourne, Melbourne, Australia; <sup>3</sup>Institut des Sciences Chimiques de Rennes, UMR6226 CNRS & Université de Rennes, Rennes, France

### FUNDAMENTALS: IONIZATION 312-325

- ThP 312 **Towards Comprehensive Molecular Dynamics Simulations of Native-Protein Charging in Electrospayed Droplets;** Michael S Cordes<sup>1</sup>; Elyssia S Gallagher<sup>1</sup>; <sup>1</sup>Baylor University, Waco, TX
- ThP 313 **Study on the Relationship between the Onset of Taylor Cone and Mass Spectrometry Signals;** Ching-Han Chang<sup>1</sup>; Pawel L. Urban<sup>1</sup>; <sup>1</sup>National Tsing Hua University, Hsinchu City, Taiwan
- ThP 314 **Revolutionizing Carbohydrate Analysis and Quantification in MALDI-MS through Rapid Freeze-Drying Droplet (RFDD) Method;** I-Chung Lu<sup>1</sup>; Xin-Wen Zhang<sup>1</sup>; Yu-Cheng Wu<sup>1</sup>; Yi-Ching Huang<sup>1</sup>; <sup>1</sup>Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan
- ThP 315 **Ion generation with fA to pA currents from unconventional configurations: dried emitter, sealed emitters, and non-polar solvents;** Ian T Ferraro<sup>1</sup>; Nicholas Allen<sup>1</sup>; Huishan Li<sup>1</sup>; Anyin Li<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of New Hampshire, Durham, NH
- ThP 316 **Investigating Electrospray Ionization using picoamp and microsecond Resolution;** Nicholas Allen<sup>1</sup>; Ian Ferraro<sup>1</sup>; Kanwal Jeet<sup>1</sup>; Anyin Li<sup>1</sup>; <sup>1</sup>University of New Hampshire, Durham, NH
- ThP 317 **Evaluation of Optimization Routines to Streamline Low-Flow LC-MS Setup and Operation;** Joshua A Silveira<sup>1</sup>; Gary A Schultz<sup>2</sup>; Matt Tsai<sup>2</sup>; Katherine Walker<sup>2</sup>; Cornelia Boeser<sup>2</sup>; Robert Van Ling<sup>2</sup>; Eloy R. Wouters<sup>2</sup>; <sup>1</sup>Thermo

## THURSDAY POSTERS

- Fisher Scientific, San Jose, CA; <sup>2</sup>ThermoFisher Scientific, San Jose, CA
- ThP 318 **Displacement current measurements to analyse charged droplets generated by electrospray ionisation (ESI) in a vacuum system;** Laura Lehmann<sup>1</sup>; Walter Wißdorf<sup>1</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany
- ThP 319 **Citrate-capped gold nanoparticle-enhanced laser desorption/ionization mass spectrometry imaging visualizes the effects of copper transporter inactivation on catecholamine metabolism;** Cole C Johnson<sup>1</sup>; Shubhrajit Roy<sup>2</sup>; Dalton Brown<sup>3</sup>; Caitlin M. Tressler<sup>3</sup>; Kristine Glunde<sup>3</sup>; Svetlana Lutsenko<sup>2</sup>; <sup>1</sup>Johns Hopkins School of Medicine, Baltimore, MD; <sup>2</sup>Johns Hopkins University School of Medicine, Physiology Department, Baltimore, Maryland; <sup>3</sup>Johns Hopkins Applied Imaging Mass Spectrometry (AIMS) Core, Baltimore city, MD
- ThP 320 **Hydrophobicity and Other Impacts of Emitters on Flow Rate and Voltage Selection of Electrospray Ionization;** Dayi Chen<sup>1</sup>; Nelum Perera<sup>1</sup>; Yanjia Zhang<sup>1</sup>; Aaron Timperman<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA
- ThP 321 **Statistical analysis of aspirated charged droplet signatures in non-summed mass spectra from various commercial LC-ESI-MS systems;** Patricia Itzenhäuser<sup>1</sup>; Chris Vico Heintz<sup>1</sup>; Adem Bulut<sup>1</sup>; Walter Wissdorf<sup>1</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany
- ThP 322 **Observation of charged ESI droplets aspirated in a Linear Ion Trap (LIT);** Adem Bulut<sup>1</sup>; David Coenen<sup>1</sup>; Thorsten Benter<sup>1</sup>; Walter Wißdorf<sup>1</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany
- ThP 323 **Droplet and Spraymode Induced Long-Term Behaviour of Analyte Signals in Electrospray MS Using Visual Spray Observation and Ion Current Measurements;** Chris Vico Heintz<sup>1</sup>; Walter Wißdorf<sup>1</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany
- ThP 324 **Investigation of the chlorine dioxide redox chemistry in ESI;** Ferdinand Max Wachter<sup>1</sup>; Hendrik Kersten<sup>1</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>University of Wuppertal, Faculty of Mathematics and Natural Sciences, Wuppertal, Germany
- ThP 325 **Protonation of analytes in ESI and matrix assisted ionization in vacuum modeled from the micro-scale to nano-scale;** Styliani Consta<sup>1</sup>; Lisa M Wingen<sup>2</sup>; Yiming Qin<sup>3</sup>; Véronique Perraud<sup>2</sup>; Barbara J. Finlayson-Pitts<sup>2</sup>; <sup>1</sup>University of Western Ontario, London, ON; <sup>2</sup>UC Irvine, Irvine; <sup>3</sup>City University of Hong Kong, Hong Kong, Hong Kong
- GC/MS: INSTRUMENTATION AND APPLICATIONS**  
326-364
- ThP 326 **Unlocking Medical Diagnostics Insights using GC-MS with Cold EI and 'WIN' Software;** Benny Neumark<sup>1</sup>; Tal Alon<sup>2,3</sup>; Oneg Elkabets<sup>1</sup>; Aviv Amirav<sup>1,4</sup>; <sup>1</sup>Tel Aviv University, Tel Aviv, Israel; <sup>2</sup>Tel-Aviv University, Tel-Aviv, Israel; <sup>3</sup>Afeka College of Engineering, Tel Aviv, Israel; <sup>4</sup>Aviv Analytical Ltd, Hod Hasharon, Israel
- ThP 327 **Novel Real Time-Analysis Methods and Instruments with In-Vacuum Electron Ionization Ion Sources;** Oneg Elkabets<sup>1</sup>; Benjamin Neumark<sup>1</sup>; Aviv Amirav<sup>1,2</sup>; <sup>1</sup>Tel Aviv University, Tel Aviv, Israel; <sup>2</sup>Aviv Analytical Ltd, Hod Hasharon, Israel
- ThP 328 **Unknown, Unexpected, and Untargeted – Illuminating the Dark Side of the Sample Using GC-MS With Cold EI;** Alex Yakovchuk<sup>1</sup>; Aviv Amirav<sup>2</sup>; <sup>1</sup>Tel Aviv University, Tel Aviv, Israel; <sup>2</sup>Tel-Aviv University, Tel-Aviv, Israel
- ThP 329 **Compact Multi Reflecting GC-TOF with High Dynamic Range;** Aleksey Vorobyev<sup>1</sup>; Yuri Khasin<sup>1</sup>; Vasily Makarov<sup>1</sup>; Anatoly Verenchikov<sup>1</sup>; <sup>1</sup>MSC-CG, Bar, Montenegro
- ThP 330 **Identification of Metabolites in Porcine Serum with Hydrogen Carrier Gas by GC/MS;** Samuel Haddad; *Agilent Technologies, Wilmington, DE*
- ThP 331 **Two Methods to Perform the New US EPA Method 1628 with GC/MSD: Traditional Helium Carrier Gas and Hydrogen Carrier Gas;** Jennifer Sanderson<sup>1</sup>; Samuel Haddad<sup>2</sup>; <sup>1</sup>Agilent Technologies, Inc., Wilmington, DE; <sup>2</sup>Agilent Technologies, Wilmington, DE
- ThP 332 **Analysis of essential oils using a comprehensive GCxGC with a reverse flow modulator combined with high resolution GC/MS;** Nick Harden<sup>1</sup>; Sofia Nieto<sup>1</sup>; Scott Hoy<sup>2</sup>; Kai Chen<sup>1</sup>; Matthew Curtis<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc., Santa Clara, CA; <sup>2</sup>Agilent Technologies, Inc., Wilmington, DE
- ThP 333 **Reducing background contamination via split mode GCMS: Accurate quantitation of palmitate enrichment for measuring in vivo lipolysis;** Zhongyuan Sun<sup>1</sup>; Allison Lau<sup>1</sup>; Gregory Tesz<sup>1</sup>; Michelle Clasquin<sup>1</sup>; <sup>1</sup>Pfizer, Cambridge, MA
- ThP 334 **Classification of Oxygen-Containing Compounds in Aviation Fuels by Using Two-Dimensional Gas Chromatography/ Methane Chemical Ionization Time-of-Flight Mass Spectrometry;** Grace Greene<sup>1</sup>; Caroline E. R. Rowell<sup>2</sup>; Michael Rees<sup>2</sup>; Jacob Guthrie<sup>3</sup>; Michael E. Peretch<sup>4</sup>; Gozdem Kilaz<sup>2,5</sup>; Hiikka I Kenttämä<sup>2</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Purdue University Department of Chemistry, West Lafayette, IN; <sup>3</sup>Naval Research Laboratory, Washington, DC; <sup>4</sup>Naval Air Warfare Center Aircraft Division (NAWCAD), Patuxent River, MD; <sup>5</sup>Purdue University, School of Engineering Technology, West Lafayette, IN
- ThP 335 **Thermal Desorption-Pyrolysis Gas Chromatography-Mass Spectrometry to Investigate the Fate of Fungicides in Window Wood Treatments;** Nafisa Bala<sup>1</sup>; Alena Kubátová<sup>1</sup>; Evguenii Kozliak<sup>1</sup>; <sup>1</sup>University of North Dakota, Grand Forks, ND
- ThP 336 **Online Catalyst Free Gas-phase Esterification of Long Chain Fatty Acids Via Gas Chromatography - Mass Spectrometry;** Alexander D. Smiarowski<sup>1</sup>; Isaac Agyekum<sup>1</sup>; <sup>1</sup>University of North Georgia, Oakwood, GA
- ThP 337 **Synthesis of tetrakis(3,5-bis(trifluoromethyl)phenyl) sodium borate as a derivatizing agent for the determination of Hg<sup>2+</sup> and CH<sub>3</sub>Hg<sup>+</sup> species by GC-TQMS/MS;** Tania Lizeth Espinoza Cruz<sup>1</sup>; Katarzyna Dorota Wrobel<sup>2</sup>; Eunice Yañez-Barrientos<sup>2</sup>; Alma Rosa Corrales-Escobosa<sup>2</sup>; Israel Enciso-Donis<sup>2</sup>; Oracio Serrano-Torres<sup>1</sup>; Antonio de Jesus Gomez-Infante<sup>2</sup>; Sergio Lopez-Azpeitia<sup>1</sup>; Kazimierz Wrobel<sup>2</sup>; <sup>1</sup>University of Guanajuato, Guanajuato, Mexico; <sup>2</sup>University of Guanajuato, Guanajuato, Mexico
- ThP 338 **Improving identification of untargeted GC/MS EI spectra with new library-based spectral and retention index analysis methods;** Deborah F. McGlynn<sup>1</sup>; Lindsay D. Yee<sup>2</sup>; Lewis Y. Geer<sup>1</sup>; Yuri A Mirokhin<sup>1</sup>; Dmitrii V Tchekhovskoi<sup>1</sup>; Coty N. Jen<sup>3</sup>; Allen H. Goldstein<sup>2</sup>; Anthony J. Kearsley<sup>1</sup>; Stephen E Stein<sup>1</sup>; <sup>1</sup>National Institute for Standards and Technology, Gaithersburg, MD; <sup>2</sup>University of California, Berkeley, Berkeley; <sup>3</sup>Carnegie Mellon University, Pittsburgh, Pennsylvania
- ThP 339 **Measurement of Polycyclic Aromatic Hydrocarbons in Complex Samples using Gas Chromatography with Pseudo MS/MS: Reduction of Potential Interferences;** Bruce A. Benner<sup>1</sup>; Walter B. Wilson<sup>1</sup>; Lane C. Sander<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD
- ThP 340 **Software Assisted Manual Evaluation for Expanding an Electron Ionization Mass Spectral Library;** Weihua Ji<sup>1</sup>; Yufang Zheng<sup>1</sup>; H Martin Garraffo<sup>1</sup>; William E. Wallace<sup>1</sup>; Stephen E. Stein<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD
- ThP 341 **Analysis of Volatile Organic Compounds in Indoor Air Using Diffusive Sorbent Pen and In-Oven Capillary GC Column Focusing;** Weier Hao<sup>1</sup>; VICTORIA VOGEL<sup>1</sup>; Dan Cardin<sup>1</sup>; <sup>1</sup>Entech Instruments, Simi Valley, CA
- ThP 342 **Analysis of Volatile and Semivolatile Organic Compounds in Food Products and Packaging using Flash Vacuum Assisted Sorbent Extraction;** Daniel Cardin<sup>1</sup>; VICTORIA VOGEL<sup>1</sup>; Weier Hao<sup>1</sup>; <sup>1</sup>Entech Instruments, Simi Valley, CA
- ThP 343 **Full Evaporative Vacuum Extraction (FEVE) – Quantitation of SVOC Contaminants per EPA Method 525 by GC-MS in Drinking Water Matrices;** VICTORIA VOGEL<sup>1</sup>; Daniel B. Cardin<sup>1</sup>; Weier Hao<sup>1</sup>; <sup>1</sup>Entech Instruments, Simi Valley, CA

## THURSDAY POSTERS

- ThP 344 **Higher Sensitivity Exploris GC Platform for Environmental and Food Analysis;** Mikhail Belov<sup>1</sup>; Brody Guckenberger<sup>2</sup>; Lothar Rottmann<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific (Bremen), Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific, Austin, Texas; <sup>3</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- ThP 345 **Solvent-free automated thermal desorption coupled online to gas chromatography/mass spectrometry for direct screening of foreign chemicals in consumer textiles;** Tim Åström<sup>1</sup>; Josefina Carlsson<sup>1</sup>; Ulrika Nilsson<sup>1</sup>; Conny Östman<sup>1</sup>; <sup>1</sup>Stockholm University, Stockholm, Sweden
- ThP 346 **What's in your water!;** Ashish Chaudhary<sup>1</sup>; Dustin McRae<sup>1</sup>; <sup>1</sup>Detect-ION, Tampa, FL
- ThP 347 **Ensuring food safety through the study of potential extractables and leachables in roasted coffee packaging by ultra-sensitive Headspace GC-MS;** Ana Caroline Martimiano<sup>1</sup>; Rodrigo Ossamu Saga Kitamura<sup>1</sup>; Isabela de Oliveira e Silva<sup>1</sup>; Ricardo Tamashiro Reis<sup>1</sup>; <sup>1</sup>Shimadzu do Brasil, Barueri, Brazil
- ThP 348 **Mining LC Fractions of Natural Product Mixtures for Complementary Data Using "Shotgun" APGC-MS;** Jeffrey Morre<sup>1</sup>; Parker Rianda<sup>1</sup>; Jaewoo Choi<sup>1</sup>; Jan F. Stevens<sup>1</sup>; Claudia S. Maier<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR
- ThP 349 **Composition Identification and Pyrolysis Mechanism of Flame-Retardant Acrylic Fabrics Investigated by Pyrolysis-Gas Chromatography-Mass Spectrometry;** Junyan Liu<sup>1</sup>; Han Xiao<sup>1</sup>; Jiyou Shi<sup>1</sup>; Jiangli Li<sup>1</sup>; Yuhong Zhang<sup>1</sup>; <sup>1</sup>Sinopec Shanghai Research Institute of Petrochemical Technology Co. Ltd., Shanghai, China
- ThP 350 **Reducing the Pain Point of GC Retention Index Calibration for Enhanced GC/MS Compound Identification;** Don Kuehl<sup>1</sup>; Stacey C. Simonoff<sup>2</sup>; Yongdong Wang<sup>2</sup>; <sup>1</sup>Cerno Bioscience, Las Vegas, NV; <sup>2</sup>Cerno Biosciences, Las Vegas, NV
- ThP 351 **Advancing Product Safety: Determination of trace Benzene in Cosmetic Products using Headspace Gas Chromatography tandem triple quadrupole mass spectrometry (GC-MS/MS);** Pei-Yi Yvonne Chee<sup>1</sup>; Chee-Leong Kee<sup>1</sup>; Nuan-Ping Cheah<sup>1</sup>; Huishi Koh<sup>1</sup>; <sup>1</sup>Health Sciences Authority, Singapore, Singapore
- ThP 352 **Exploiting GC(xGC)-HRMS capabilities for targeted and non-targeted analysis of (semi)volatile poly- & perfluorinated hydrocarbons in ambient air;** Maria Chiara Corvisieri<sup>1</sup>; Marco De Poli<sup>2</sup>; Claudia Stevanin<sup>1</sup>; Tatiana Chenet<sup>1</sup>; Alberto Cavazzini<sup>2</sup>; Luisa Pasti<sup>1</sup>; Flavio Antonio Franchina<sup>2</sup>; <sup>1</sup>Department of Environmental and Prevention Sciences, University of Ferrara, Ferrara, Italy; <sup>2</sup>Department of Chemical, Pharmaceutical, and Agricultural Sciences, University of Ferrara, Ferrara, Italy
- ThP 353 **Meeting the challenges of Dioxin analysis and more with GC-Orbitrap high mass resolution capabilities;** Dominic Roberts<sup>1</sup>; Nicholas Warner<sup>2</sup>; Paolo Benedetti<sup>3</sup>; Xin Zheng<sup>4</sup>; Jason Cole<sup>4</sup>; Daniel Kutscher<sup>5</sup>; <sup>1</sup>Thermo Fisher Scientific, Runcorn, United Kingdom; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific, Milan, Italy; <sup>4</sup>Thermo Fisher Scientific, Austin, Texas; <sup>5</sup>Thermo Fisher Scientific, Bremen, Germany
- ThP 354 **Improved identification of extractable and leachable substances with Orbitrap Exploris GC 240;** Dominic Roberts<sup>1</sup>; Nicholas Warner<sup>2</sup>; Xin Zheng<sup>3</sup>; Jason Cole<sup>3</sup>; Duijuan Lu<sup>4</sup>; Chongming Liu<sup>4</sup>; Nan Zhang<sup>4</sup>; Sven Hackbusch<sup>5</sup>; Daniel Kutscher<sup>6</sup>; <sup>1</sup>Thermo Fisher Scientific, Runcorn, United Kingdom; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific, Austin, Texas; <sup>4</sup>SGS Health Science, Fairfield, New Jersey; <sup>5</sup>Thermo Fisher Scientific, San Jose, CA; <sup>6</sup>Thermo Fisher Scientific, Bremen, Germany
- ThP 355 **Comparison of Different Sample Preparation Techniques for Analyzing Volatile and semi-Volatile Organic Compounds in Recycled Plastics Using GC/MS;** Renzo Picononi<sup>1</sup>; Tiantian Li<sup>1</sup>; Günter Böhm<sup>1</sup>; Stefan Cretnik<sup>1</sup>; <sup>1</sup>CTC Analytics AG, Zwingen, Switzerland
- ThP 356 **Determination of six aromatic amines in the mainstream smoke of tobacco products;** Huihua Ji<sup>1</sup>; Zhenyu Jin<sup>1</sup>; <sup>1</sup>University of Kentucky, Lexington, KY
- ThP 357 **Predicting Arrhenius Parameters for the Gas-Phase Decomposition of VX Using a Bench Scale Py-GC/MS System with an In-Line Reactor;** Jeffrey Michael McGuire<sup>1</sup>; John Carpin<sup>2</sup>; <sup>1</sup>U.S. Army CCDEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; <sup>2</sup>EXCET Incorporated, Edgewood, MD
- ThP 358 **Rapid Screening of Illegal Aniline Additives in Gasoline by Gas Chromatography Electrostatic Field Orbit Trap High Resolution Mass Spectrometry;** Liyan Jiang; Sinopec Shanghai Research Institute of Petrochemical Technology Co. Ltd., Shanghai, China
- ThP 359 **Faster Qualitative Analysis of Essential Oils Using GC/MS with Hydrogen Carrier Gas and a Hydrogen Optimized EI Source;** Bruce Quimby<sup>1</sup>; Anastasia Andrianova<sup>1</sup>; Lakshmi Krishnan<sup>2</sup>; <sup>1</sup>Agilent Technologies, Wilmington, DE; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- ThP 360 **Fast Analysis of 140 Pesticides, PAHs, and PCBs by GC/MS/MS;** Erinn M O'Neill<sup>1</sup>; Alexis Willey<sup>1</sup>; Marta Venier<sup>2</sup>; <sup>1</sup>Agilent Technologies, Wilmington, DE; <sup>2</sup>Indiana University, Bloomington, IN
- ThP 361 **Improving Emissivity Through Improved Yttria Coatings for GCMS Filaments;** Ron Shomo<sup>1</sup>; Kenneth Wright<sup>1</sup>; <sup>1</sup>IMI ADAPTAS, Palmer, MA
- ThP 362 **Brewing Excellence: Quantitating Over 200 Pesticides in Black Tea with Steady Performance and Maximized Uptime;** Anastasia Andrianova<sup>1</sup>; Eric Fausett<sup>1</sup>; Bruce Quimby<sup>1</sup>; Limian Zhao<sup>1</sup>; Joel Ferrer<sup>2</sup>; Aaron Boice<sup>2</sup>; <sup>1</sup>Agilent Technologies, Wilmington, DE; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- ThP 363 **Enhanced Longevity and Revolutionized Robustness for Sensitive Detection of 190 Pesticides over 800 Injections with Novel HES 2.0 Source;** Brooke C Reaser<sup>1</sup>; Luis Cuadra-Rodriguez<sup>1</sup>; Elias Feresenbet<sup>1</sup>; Ge Yu<sup>1</sup>; Alexander Mordehai<sup>1</sup>; Nathan Eno<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- ThP 364 **Novel High Sensitivity Detector for GC/MS;** Hiroki Kanno<sup>1</sup>; Shun Kogiso<sup>2</sup>; Yoshiro Hiramatsu<sup>3</sup>; Alan Owens<sup>3</sup>; Masaru Nishiguchi<sup>2</sup>; <sup>1</sup>Shimadzu, Kyoto, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Shimadzu Scientific Instruments, Columbia, MD

### GLYCOPROTEINS II 365-393

- ThP 365 **Mass spectrometry-based structure-specific N-glycoproteomics and applications;** Zhixin Tian; Department of Chemistry, Tongji University, Shanghai, China
- ThP 366 **Systematic investigation of the trafficking of glycoproteins on the cell surface;** Xing Xu<sup>1</sup>; Kejun Yin<sup>1</sup>; Ronghu Wu<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA
- ThP 367 **Mass Spectrometric Investigation of the Fragile X Glycoproteome in Developing Mice;** Elliot Patrenets<sup>1</sup>; Hannah N Miles<sup>2</sup>; Thao Duong<sup>3</sup>; Ashley Phetsanhad<sup>3</sup>; Pamela R Westmark<sup>4,5</sup>; Cara J Westmark<sup>4,5</sup>; Lingjun Li<sup>2,3,5</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Integrative Biology, Madison, Wisconsin; <sup>2</sup>University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin; <sup>3</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, WI; <sup>4</sup>University of Wisconsin Madison, Department of Neurology, Madison, Wisconsin; <sup>5</sup>University of Wisconsin Madison, Molecular Environmental Toxicology Center, Madison, Wisconsin
- ThP 368 **Ultra-sensitive platelet proteome identifies a new form of domain-specific O-fucosylation generated by FUT10 and FUT11;** Huilin Hao<sup>1</sup>; Callum B Houlahan<sup>2</sup>; Yvonne Kong<sup>2</sup>; Michelle Cielesh<sup>2</sup>; Youxi Yuan<sup>1</sup>; Atsuko Ito<sup>1</sup>; Benjamin M Eberand<sup>2</sup>; The Huong Chau<sup>3</sup>; Morten Thaysen-Andersen<sup>3</sup>; Freda H Passam<sup>2</sup>; Robert S Haltiwanger<sup>1</sup>; Mark Larance<sup>2</sup>; <sup>1</sup>Complex Carbohydrate Research Center, Department of Biochemistry and Molecular Biology, University of Georgia,

## THURSDAY POSTERS

- Athens, GA; <sup>2</sup>The University of Sydney, Camperdown, Australia; <sup>3</sup>Macquarie University, North Ryde, Australia
- ThP 369 **Nanoflow liquid chromatography separation to enhance glycopeptide characterization;** David Colquhoun<sup>1</sup>; Patrick Pribil<sup>2</sup>; Jeremy Potriquet<sup>3</sup>; Edward Kerr<sup>4</sup>; Amanda Nouwens<sup>5</sup>; Susan Briscoe<sup>4</sup>; Tony Vuocolo<sup>4</sup>; <sup>1</sup>Sciex, Framingham, MA; <sup>2</sup>SCIEX, Concord, ON; <sup>3</sup>SCIEX, Mulgrave, Australia; <sup>4</sup>CSIRO, Brisbane, Australia; <sup>5</sup>University of Queensland, Brisbane, Australia
- ThP 370 **Deep sequencing entire glycoproteins with Proteinase K to inform HIV vaccine development;** Sabyasachi Baboo<sup>1</sup>; Jolene K. Diedrich<sup>1</sup>; Jon M. Steichen<sup>1</sup>; Torben Schiffner<sup>1</sup>; Kimmo Rantalainen<sup>1</sup>; Olivia Swanson<sup>1</sup>; Christopher A Cottrell<sup>1</sup>; Oleksandr Kalyuzhnyi<sup>1</sup>; Alessia Liguori<sup>1</sup>; William R Schief<sup>1</sup>; James C Paulson<sup>1</sup>; John R. Yates III<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA
- ThP 371 **Fragmentation Features of Electronic Excitation Dissociation Tandem Mass Spectra Useful for Accurate Glycosylation Analysis;** Nafisa Tursumamat<sup>1</sup>; Shengyang Liu<sup>1</sup>; Ruijing Li<sup>1</sup>; Shuhong Guo<sup>1</sup>; Chaoshuang Xia<sup>2</sup>; Joseph Zaia<sup>2</sup>; Catherine E. Costello<sup>2</sup>; Lin Cheng<sup>2</sup>; Juan Wei<sup>1</sup>; <sup>1</sup>School of Pharmaceutical Sciences, Shanghai Jiao Tong University, Shanghai, China; <sup>2</sup>Center for Biomedical Mass Spectrometry, Boston University Chobanian & Avedisian School of Medicine, Boston, USA, MA
- ThP 372 **Towards MS-based identification and quantification of glycopeptide isomers;** Joshua C.L. Maliepaard<sup>1,2</sup>; Karli R. Reiding<sup>1, 2</sup>; <sup>1</sup>Utrecht University, Utrecht, Netherlands; <sup>2</sup>Netherlands Proteomics Center, Utrecht, Netherlands
- ThP 373 **Reversible Enrichment of O-GlcNAcylated Glycopeptides;** Hongqiang Qin; *Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*
- ThP 374 **Quantitative Evaluation of Affimer and Molecular Imprinted Polymer Affinity Glycoproteins Analysis by Multiple Reaction Monitoring LC-MS/MS;** Billy Molloy<sup>1</sup>; Christian Tiede<sup>2</sup>; Lewis Adams<sup>2</sup>; Darren Tomlinson<sup>2</sup>; Oliver Huseyin<sup>3</sup>; Francesco Canfarotta<sup>4</sup>; Alan Thomson<sup>3</sup>; Johannes Vissers<sup>1</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>School of Molecular and Cellular Biology, University of Leeds, Leeds, United Kingdom; <sup>3</sup>MIP Discovery, Sharnbrook, United Kingdom; <sup>4</sup>MIP Discovery, Sharnbrook, United Kingdom
- ThP 375 **In vivo comprehensive profiling of the murine Galnt3-specific O-glycoproteome;** Kruti Dalal<sup>1</sup>; Weiming Yang<sup>1</sup>; E Tian<sup>2</sup>; Aliona Chernish<sup>1</sup>; Peggy McCluggage<sup>1</sup>; Kelly G Ten Hagen<sup>2</sup>; Lawrence A. Tabak<sup>1</sup>; <sup>1</sup>Biological Chemistry Section, National Institute of Dental and Craniofacial Research, National Institutes of Health, Bethesda, MD; <sup>2</sup>Developmental Glycobiology Section, National Institute of Dental and Craniofacial Research, National Institutes of Health, Bethesda, MD
- ThP 376 **Mass Spectrometry Comparison of N-linked Glycosylation on Influenza A(H3N2) Hemagglutinin in A549 and MDCK Cell lines;** Betlehem Mekonnen<sup>1</sup>; Irina Alymova<sup>2</sup>; Ian York<sup>2</sup>; Dongxia Wang<sup>1</sup>; John R Barr<sup>1</sup>; <sup>1</sup>CDC, Chamblee, GA; <sup>2</sup>CDC, Atlanta, GA
- ThP 377 **Modifying In Silico Peptide Libraries to Facilitate N-Glycopeptide Real-Time Library Searching;** Kathryn Kothlow<sup>1</sup>; Anna G. Duboff<sup>1</sup>; Jacob H. Russell<sup>1</sup>; Emmajay Sutherland<sup>1</sup>; Nicholas M. Riley<sup>1</sup>; <sup>1</sup>University of Washington, Seattle
- ThP 378 **Real-time searching for truncated N-glycopeptides following Endo-H treatment;** Anna G. Duboff<sup>1</sup>; Kathryn Kothlow<sup>1</sup>; Jacob H. Russell<sup>1</sup>; Emmajay Sutherland<sup>1</sup>; Nicholas M. Riley<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- ThP 379 **Expansion of Autonomous-Type Dissociation Selection to Include Core-2 O-Glycopeptides for Improved Characterization of O-Glycopeptides;** Jacob H. Russell<sup>1</sup>; Emmajay Sutherland<sup>1</sup>; Ruby Zhang<sup>1</sup>; Nicholas M. Riley<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- ThP 380 **Comprehensive LC-PAD/MS Analysis of N-glycans using SweetSep™ HPAEC Column;** Christian Marvelous<sup>1</sup>; Jean-Pierre Chervet<sup>1</sup>; Hendrik-Jan Brouwer<sup>1</sup>; Martin Eysberg<sup>2</sup>; Valentina Valentini<sup>2</sup>; <sup>1</sup>Antec Scientific, Alphen aan den Rijn, Netherlands; <sup>2</sup>Antec Scientific, Boston, MA
- ThP 381 **Veneer is a webtool for rapid, standardized, and transparent interpretation, annotation, and reporting of mammalian cell surface N-glycocapture data;** Linda Berg Luecke<sup>1, 2</sup>; Roneldine Mesidor<sup>1</sup>; Jack Littrel<sup>1</sup>; Morgan Carpenter<sup>1</sup>; Melinda Wojtkiewicz<sup>1</sup>; Rebekah L Gundry<sup>1</sup>; <sup>1</sup>University of Nebraska Medical Center, Omaha, NE; <sup>2</sup>Medical College of Wisconsin, Milwaukee, WI
- ThP 382 **Introducing DIA Glycoproteomics Analysis in FragPipe;** Daniel Polasky<sup>1</sup>; Fengchao Yu<sup>1</sup>; Weiming Yang<sup>2</sup>; Guo Ci Teo<sup>1</sup>; Yan Wang<sup>3</sup>; Alexey I. Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Section on Biological Chemistry, National Institute of Dental and Craniofacial Research (NIDCR), NIH, Bethesda, MD; <sup>3</sup>Mass Spectrometry Facility, NICDR, NIH, Bethesda, MD
- ThP 383 **Proton Transfer Charge Reduction to Investigate Co-isolation in Glycoproteomics;** Kayla Markuson<sup>1</sup>; Ruby Zhang<sup>1</sup>; Nicholas M. Riley<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- ThP 384 **N-Glycoproteome of Brain Tissue from the Frontal Lobe is Altered During the Development and Progression of Parkinson's Disease;** Oluwatosin E Daramola<sup>1</sup>; Judith Nwaiwu<sup>2</sup>; Joy Solomon<sup>2</sup>; Moyinoluwa Adeniyi<sup>2</sup>; Andrew I. Bennett<sup>2</sup>; Yehia Mechref<sup>2</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>Texas Tech University, Lubbock, Texas
- ThP 385 **Exploring N-glycoproteome characterization with the Orbitrap Astral Mass Spectrometer;** Annie Jen<sup>1</sup>; Noah M. Lancaster<sup>1,2</sup>; Katherine A. Overmyer<sup>1, 3, 4</sup>; Scott T. Quarmby<sup>1</sup>; Daniel A. Polasky<sup>5</sup>; Alexey I. Nesvizhskii<sup>5</sup>; Joshua J. Coon<sup>1, 2, 3, 4</sup>; <sup>1</sup>Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>Morgridge Institute for Research, Madison, WI; <sup>4</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI; <sup>5</sup>University of Michigan, Ann Arbor, MI
- ThP 386 **Isomeric Separation of O-Glycopeptides and Glycosylated Isoforms from Standard Glycoproteins Utilizing Mesoporous Graphitic Carbon (MGC) Material and Tandem MS;** Cristian D Gutierrez-Reyes<sup>1</sup>; Oluwatosin Daramola<sup>2</sup>; Mojibola Fowowe<sup>2</sup>; Sherifdeen B Onigbinde<sup>2</sup>; Judith Ijeoma Nwaiwu<sup>2</sup>; Vishal Sandilya<sup>2</sup>; Yehia Mechref<sup>2</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>Texas Tech University, Lubbock, Texas
- ThP 387 **Glycoproteomics of ER-Stress in Cardiomyocytes;** Alexander W Black<sup>1, 2</sup>; Boomathi Pandi<sup>1</sup>; Cheyanne Durham<sup>1</sup>; Dominic C.M. Ng<sup>1</sup>; Maggie P.Y. Lam<sup>1, 2, 3</sup>; <sup>1</sup>Department of Medicine/Division of Cardiology, University of Colorado School of Medicine, Aurora, CO; <sup>2</sup>Department of Biochemistry and Molecular Genetics, Aurora, CO; <sup>3</sup>Consortium for Fibrosis Research and Translation (CFReT), Aurora, CO
- ThP 388 **Label-free quantification of serum glycopeptides reveals novel biomarkers for advanced colorectal adenoma;** Gege Xu<sup>1</sup>; Rachel Rice<sup>1</sup>; Maryam Baniasad<sup>1</sup>; Ranjan Dalao-Bhadra<sup>1</sup>; Itati Hundal<sup>1</sup>; Gregg Czerwiec<sup>1</sup>; Xin Cong<sup>1</sup>; <sup>1</sup>InterVenn Biosciences, South San Francisco, CA
- ThP 389 **Reproducible enrichment of N-glycopeptides with HPLC Fractionation;** Rachel Rice<sup>1</sup>; Gege Xu<sup>2</sup>; Hector Huang<sup>2</sup>; Maryam Baniasad<sup>2</sup>; Ranjan Bhadra<sup>2</sup>; Xin Cong<sup>2</sup>; <sup>1</sup>InterVenn Biosciences, South San Francisco, CA; <sup>2</sup>InterVenn Biosciences, South San Francisco, CA
- ThP 390 **Site-specific analysis of co-occupied N- and O-glycopeptides;** Joann Chongsaritsinsuk<sup>1</sup>; Valentina Rangel-Angarita<sup>1</sup>; Keira E. Mahoney<sup>1</sup>; Stacy A. Malaker<sup>1</sup>; <sup>1</sup>Yale University, New Haven, CT
- ThP 391 **Glycopeptide Enrichment through an All-biomass Synthesized Carbon Nanofiber Aerogel;** Haoran Zhang<sup>1</sup>; Wenxin Wu<sup>1</sup>; Lingjun Li<sup>1, 2</sup>; <sup>1</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin; <sup>2</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin

## THURSDAY POSTERS

- ThP 392 **Exploring Site-Specific Glycosylation of Band 3 Protein in Human and Transgenic Porcine Erythrocytes for Xenotransfusion Comparability;** Jae Ho Kim<sup>1,2</sup>; Myung Jin Oh<sup>1,2</sup>; Jong Shin Yoo<sup>1,2</sup>; Joohyun Shim<sup>3</sup>; Kimyung Choi<sup>3</sup>; Hyun Joo An<sup>1,2</sup>; <sup>1</sup>Chungnam National University, Daejeon, South Korea; <sup>2</sup>Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; <sup>3</sup>Optipharm Inc., Cheongju, South Korea
- ThP 393 **Fragment ion triggered Parallel Accumulation SERIAL Fragmentation stepping for enhanced glycoproteomics data acquisition;** Gad Armony<sup>1</sup>; Michael Krause<sup>2</sup>; Pierre-Olivier Schmit<sup>3</sup>; Dennis Trede<sup>2</sup>; Gary Kruppa<sup>4</sup>; Dirk Lefebvre<sup>1,5</sup>; Alain Van Gool<sup>1</sup>; Hans Wessels<sup>6</sup>; <sup>1</sup>Translational Metabolic Laboratory, Department of genetics, Radboud University Medical Center, Nijmegen, Netherlands; <sup>2</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany; <sup>3</sup>Bruker Daltonique S.A., Wissembourg, France; <sup>4</sup>Bruker S.R.O., Brno, Czech Republic; <sup>5</sup>Department of Neurology, Donders Institute for Brain, Cognition, and Behavior, Radboud University Medical Center, Nijmegen, Netherlands; <sup>6</sup>Radboudumc, Nijmegen, Netherlands
- HIGH MASS ACCURACY/HIGH PERFORMANCE MS:  
APPLICATIONS  
394-412**
- ThP 394 **Unveiling Complexities: Integration of Ion Mobility and Charge-Detection Mass Spectrometry for the Analysis of Multimeric Complexes;** Kyle Juetten<sup>1</sup>; James Sanders<sup>2</sup>; Michael Marty<sup>2</sup>; Jennifer Brodbelt<sup>1</sup>; <sup>1</sup>University of Texas at Austin, Austin, TX; <sup>2</sup>University of Arizona, Tucson, AZ
- ThP 395 **Improved Mass Accuracy and Precision for MAM using a New Internally Calibrated High Resolution Orbitrap Mass Detector;** Andrew William Dawdy<sup>1</sup>; Edna A Trujillo<sup>1</sup>; Zhenjiu Liu<sup>1</sup>; Julia Kraegenbring<sup>2</sup>; Catharina Crone<sup>2</sup>; Kai Scheffler<sup>3</sup>; <sup>1</sup>Pfizer, Chesterfield, MO; <sup>2</sup>Thermo Fisher Scientific GmbH, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific, Germering, Germany
- ThP 396 **Automating Analysis of 1536-well nano-scale High Throughput Environment (HTE) experiments via acoustic ejection high resolution mass spectrometry;** Neal Liddle<sup>1</sup>; Chang Liu<sup>2</sup>; Nomaan Rezayee<sup>1</sup>; Shane Yost<sup>1</sup>; James Garrafa<sup>1</sup>; Joanna Vo<sup>1</sup>; Fred Manby<sup>1</sup>; Mark Spears<sup>3</sup>; Tom Covey<sup>2</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>Iambic Therapeutics, San Diego, CA; <sup>2</sup>SCIEX, Concord, ON; <sup>3</sup>Virscidian, Inc, Cary, NC
- ThP 397 **APCI-MS for the analysis of cultural heritage materials;** Anu Teearu-Ojakäär<sup>1</sup>; Signe Vahur<sup>1</sup>; <sup>1</sup>University of Tartu, Institute of Chemistry, Tartu, Estonia
- ThP 398 **Evaluation of the NIST library matching quality of mass spectra generated by the GC-HR-TOFMS with Multi-Mode Ionization Source;** Craig Fowler<sup>1</sup>; Scott Pugh<sup>1</sup>; George Tikhonov<sup>1</sup>; Slava Artaev<sup>1</sup>; <sup>1</sup>LECO, St. Joseph, MI
- ThP 399 **Charting New Paths in Lipidomics: An Evaluation of DDA and DIA on an Astral Mass Spectrometer;** Salma I. Abouelhassan<sup>1</sup>; Katherine A Overmyer<sup>1, 2, 3</sup>; Benton J Anderson<sup>1, 3</sup>; Scott T Quarmby<sup>1, 3</sup>; Joshua J Coon<sup>1, 2, 3, 4</sup>; <sup>1</sup>Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Morgridge Institute for Research, Madison, WI; <sup>3</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI; <sup>4</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- ThP 400 **Identification and Quantitation of Low-MW Dendrimer (10183 Da) in Rat Plasma Using QExactive Mass Spectrometry (QE-MS);** Gabriel Velazquez<sup>1</sup>; Troy Voelker<sup>2</sup>; Brandon Wilcock<sup>2</sup>; Emily Clement<sup>3</sup>; Rémy Poupot<sup>4</sup>; Cédric-Olivier Turrin<sup>3</sup>; <sup>1</sup>Aliri Bioanalysis, Millcreek, UT; <sup>2</sup>Aliri Bioanalysis, Salt Lake City, UT; <sup>3</sup>IMD-Pharma, Toulouse, France; <sup>4</sup>Université de Toulouse, Toulouse, France
- ThP 401 **Development of the high sensitivity and high resolution post processing methods for biopharmaceutical analyses with multi-turn TOF-MS;** Yusuke Tateishi<sup>1</sup>; Hiroko Morinaga<sup>1</sup>; Hiroyuki Miura<sup>1</sup>; Koichi Kimura<sup>1</sup>; Masaru Nishiguchi<sup>1</sup>; Atsuhiko Toyama<sup>1</sup>; Osamu Furuhashi<sup>1</sup>; Daisuke Okumura<sup>1</sup>; Tairo Ogura<sup>2</sup>; Yuki Yamaguchi<sup>3</sup>; Susumu Uchiyama<sup>3</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>3</sup>Osaka university, Osaka, Japan
- ThP 402 **Intercomparison Study of two High-Resolution TOF-MS for Ultra-Trace Detection;** Lena Marie Mokros<sup>1</sup>; Niklas Pengemann<sup>1</sup>; Hendrik Kersten<sup>1</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany
- ThP 403 **Maximizing the output in metabolomics - Combining high-speed DDA and MRM for simultaneous absolute quantification and non-targeted screening;** Lisa Panzenboeck<sup>1,2</sup>; Harald Schoeny<sup>1</sup>; Bruno Stelzer<sup>1</sup>; Elisabeth Foels<sup>1, 2</sup>; Marlene Puehringer<sup>1, 2</sup>; Dorian Hirschmann<sup>3</sup>; Christian Dorfer<sup>3</sup>; Daniela Loetsch<sup>3</sup>; Gunda Koellensperger<sup>1, 4</sup>; <sup>1</sup>Department of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria; <sup>2</sup>Vienna Doctoral School in Chemistry (DoSChem), University of Vienna, Vienna, Austria; <sup>3</sup>Department of Neurosurgery, Medical University Vienna, Vienna, Austria; <sup>4</sup>Vienna Metabolomics Center (VIME), University of Vienna, Vienna, Austria
- ThP 404 **High Resolution Ion Mobility and Ultra-High resolution mass spectrometry for DOM chemical Formula based Structural Assignment;** Pablo R B Oliveira<sup>1</sup>; Denny Leyva<sup>1</sup>; Lilian V Tose<sup>1</sup>; Muhammad U Tariq<sup>1</sup>; Chad Weisbrod<sup>2</sup>; Fahad Saeed<sup>1</sup>; Francisco A Fernandez-Lima<sup>1</sup>; <sup>1</sup>Florida International University, Miami, FL; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL
- ThP 405 **Exploring Ion Coalescence in Orbitrap Mass Spectrometry: A Comparative Study with PFAS Compounds 6:2 FTS and Hydro-EVE;** Jeffrey Enders; North Carolina State University, Raleigh, NC
- ThP 406 **INTEGRATION OF TANDEM HIGH RESOLUTION ION MOBILITY AND MASS SPECTROMETRY FOR COMPLEX MIXTURE ANALYSIS;** Andrew R Forero<sup>1</sup>; Miguel Santos<sup>1</sup>; Pablo R B Oliveira<sup>1</sup>; Kevin J. De Fouque<sup>1</sup>; Cullen Greer<sup>2</sup>; Brian H Clowers<sup>2</sup>; Anton N. Kozhinov<sup>3</sup>; Yury Tsybin<sup>3</sup>; Chad R Weisbrod<sup>4</sup>; Fahad Saeed<sup>5</sup>; Francisco A Fernandez-Lima<sup>1, 6</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, Florida International University, Miami, FL; <sup>2</sup>Department of Chemistry, Washington State University, Pullman, WA; <sup>3</sup>Spectroswiss, Lausanne, Switzerland; <sup>4</sup>National High Magnetic Field Laboratory, Tallahassee, Florida; <sup>5</sup>Knight Foundation School of Computing and Information Sciences, Florida International University, Miami, FL; <sup>6</sup>Biomolecular Sciences Institute, Florida International University, Miami, FL
- ThP 407 **Characterization of Monoclonal Antibody (mAbs) using Shimadzu Q-TOF LCMS 9030;** Shannie Tav<sup>1</sup>; Max Kosok<sup>1</sup>; <sup>1</sup>Shimadzu (Asia Pacific), Singapore, Singapore
- ThP 408 **Assessment of High-Resolution DIA Methods and Short Gradients on High-Throughput µPAC Columns for Maximum Proteome Coverage and Quantitative Performance;** Julia Kraegenbring<sup>1</sup>; Dominic G. Hoch<sup>2</sup>; Jeff Op De Beeck<sup>3</sup>; Riccardo Stucchi<sup>2</sup>; Hanno Resemann<sup>1</sup>; Robert Van Ling<sup>3</sup>; Heiner Koch<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific, Reinach, Switzerland; <sup>3</sup>Thermo Fisher Scientific, Ghent, Belgium
- ThP 409 **From Rough Signal to Polished Spectrum: Absorption Mode Two-dimensional Mass Spectrometry;** Maria Van Agthoven<sup>1</sup>; Sarah V Heel<sup>2</sup>; Marek Polak<sup>3,4</sup>; Alan Kadek<sup>3</sup>; Petr Novak<sup>3, 4</sup>; Kathrin Breuker<sup>2</sup>; Carlos Afonso<sup>1</sup>; Marc-André Delsuc<sup>5</sup>; <sup>1</sup>University of Rouen-Normandy, Mont-Saint-Aignan, France; <sup>2</sup>University of Innsbruck, Innsbruck, Austria; <sup>3</sup>BioCeV – Institute of Microbiology, The Czech Academy of Sciences, Prague, Czech Republic; <sup>4</sup>Charles University, Prague, Czech Republic; <sup>5</sup>IGBMC Gie CERBM, ILLKIRCH CEDEX, France
- ThP 410 **Advances in Absorption Mode FT-ICR Mass Spectral Quality with MagLab Predator Data Acquisition and Analysis Software;** Greg T Blakney<sup>1</sup>; Amy M McKenna<sup>1</sup>; Chad R Weisbrod<sup>1</sup>; Steve C. Beu<sup>2</sup>; Christopher L Hendrickson<sup>1</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, Florida; <sup>2</sup>S C Beu Consulting, Austin, TX
- ThP 411 **Metaproteomics optimization on Thermo Astral and Fusion mass spectrometers;** Matthew McIlvin<sup>1</sup>; Paloma

## THURSDAY POSTERS

Lopez<sup>1</sup>; Mak Saito<sup>1</sup>; <sup>1</sup>Woods Hole Oceanographic Inst., Woods Hole, MA

- ThP 412 **Capillary Electrophoresis with Absorption Mode Fourier Transform Ion Cyclotron Resonance**; Jonathan Choi<sup>1</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA

**IMAGING MS: COMPUTATIONAL METHODS, SOFTWARE, AND ANALYSIS**  
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- ThP 413 **Metabolite-preserving single cell MALDI imaging reveals metabolite markers of microglia activation in tissue**; James Lucas Cairns<sup>1, 2</sup>; Johanna Huber<sup>1</sup>; Stefan Maurer<sup>3</sup>; Andrea Lewen<sup>4</sup>; Jessica Jung<sup>5</sup>; Stefan Schmidt<sup>1</sup>; Janne Jasmin Wiedmann<sup>6</sup>; Tobias Bausbacher<sup>1</sup>; Pavel Levkin<sup>6, 7</sup>; Philipp Koch<sup>5, 8</sup>; Kerstin Göpprich<sup>3, 9</sup>; Oliver Kann<sup>4, 10</sup>; Carsten Hopf<sup>1, 2, 5</sup>; <sup>1</sup>CeMOS, Bioanalytics, University of Applied Sciences Mannheim, Mannheim, Germany; <sup>2</sup>Medical Faculty, Heidelberg University, Heidelberg, Germany; <sup>3</sup>Biophysical Engineering Group, Max Planck Institute for Medical Research, Heidelberg, Germany; <sup>4</sup>Institute of Physiology and Pathophysiology, University of Heidelberg, Heidelberg, Germany; <sup>5</sup>Mannheim Center for Translational Neuroscience (MCTN), Mannheim, Germany; <sup>6</sup>Institute of Biological and Chemical Systems (IBCS-FMS), Karlsruhe, Germany; <sup>7</sup>Institute of Organic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany; <sup>8</sup>German Cancer Research Center, Heidelberg, Heidelberg, Germany; <sup>9</sup>Biophysical Engineering Group, Center for Molecular Biology of Heidelberg University (ZMBH), Heidelberg, Germany; <sup>10</sup>Interdisciplinary Center for Neurosciences (IZN), Heidelberg, Germany

- ThP 414 **A Machine Learning Approach to System Suitability Testing for Mass Spectrometry Imaging**; Russell R Kibbe<sup>1</sup>; Alexandria L. Sohn<sup>1</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC

- ThP 415 **Analysis of MSI data using rr2-NMF reveals detailed spectral and spatial visualization of co-localized molecules, both highly and lowly abundant**; Melanie Nijs<sup>1</sup>; Etienne Waelkens<sup>1</sup>; Bart De Moor<sup>1</sup>; <sup>1</sup>KU Leuven, Leuven, Belgium

- ThP 416 **A technology-neutral software package for integrated spatial multi omics visualization and data analysis**; Nathan Heath Patterson<sup>1</sup>; Wanqiu Zhang<sup>1</sup>; Maria José Q Mantas<sup>1</sup>; Phuong Thao Tran<sup>1</sup>; Reza R Choubeh<sup>1</sup>; Baruch Berger<sup>1</sup>; Fang Xue<sup>2</sup>; M. Reid Groseclose<sup>2</sup>; Pedro Machado Almeida<sup>3</sup>; Alice Ly<sup>1</sup>; Peter Roelants<sup>1</sup>; Thomas Moerman<sup>1</sup>; Nico Verbeeck<sup>1</sup>; Marc Claesen<sup>1</sup>; <sup>1</sup>Aspect Analytics, Genk, Belgium; <sup>2</sup>GSK, Collegeville, PA; <sup>3</sup>Lunaphore Technologies SA., Tolochenaz, Switzerland

- ThP 417 **Strategies for assessing and monitoring consistent quality in MALDI Imaging experiments**; Tanja Bien<sup>1</sup>; Ulrike Schweiger Hufnagel<sup>1</sup>; Arne Fuetterer<sup>1</sup>; Hauke Mönck<sup>1</sup>; Stefan Harsdorf<sup>1</sup>; Sergio Legaz<sup>1</sup>; Christoph Nordmann<sup>1</sup>; Corinna Henkel<sup>1</sup>; Janina Oetjen<sup>1</sup>; Nadine T. Smit<sup>1</sup>; Jan H. Kobarg<sup>1</sup>; Matthew R Lewis<sup>2</sup>; Michael Easterling<sup>3</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; <sup>2</sup>Bruker UK Limited, Life Sciences Mass Spectrometry Division, Coventry, United Kingdom; <sup>3</sup>Bruker Scientific, 40 Manning Road, Billerica, MA

- ThP 418 **Integrated MALDI-2 MS Imaging and Single-Cell Analysis for Brain Region-Specific Chemical Profiling in Alzheimer's Disease**; Timothy J Trinklein<sup>1</sup>; Stanislav S Rubakhin<sup>1</sup>; Marisa Asadian<sup>1</sup>; K.R. Rajesh<sup>2</sup>; Orly Lazarov<sup>2</sup>; Fan Lam<sup>1</sup>; Jonathan V Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois Urbana Champaign, Champaign, IL; <sup>2</sup>University of Illinois at Chicago, Chicago, IL

- ThP 419 **Integration and joint multivariate analysis of multimodal chemical imaging data on an example case of hepatocellular carcinoma in rat**; Katharina Kronenberg<sup>1</sup>; Soeren-Oliver Deininger<sup>2</sup>; Marten Seeba<sup>3</sup>; Julia Werner<sup>4</sup>; Peter Bohrer<sup>4</sup>; Rickmer F Braren<sup>4</sup>; Fabian K Lohöfer<sup>4</sup>; Heiko Neuweeger<sup>2</sup>; Uwe Karst<sup>1</sup>; <sup>1</sup>University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; <sup>2</sup>Bruker Daltonics GmbH & Co.KG, Bremen, Germany;

<sup>3</sup>Bruker Optics GmbH & Co. KG, Ettlingen, Germany; <sup>4</sup>Institute of Diagnostic and Interventional Radiology, School of Medicine, Technical University of Munich, Munich, Germany

- ThP 420 **Automated Isotope Detection in Imaging Mass Spectrometry Through Spatial and Spectral Cues**; Meenakshi Meenakshi<sup>1</sup>; Lukasz Migas<sup>1</sup>; Katerina V. Djambazova<sup>2, 3</sup>; Martin Dufresne<sup>2, 4</sup>; Jeffrey M Spraggins<sup>2, 3, 4, 5, 6</sup>; Raf Van De Plas<sup>1, 2, 4</sup>; <sup>1</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>2</sup>Mass Spectrometry Research Center, Nashville, TN; <sup>3</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>4</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>5</sup>Department of Chemistry, Vanderbilt University, Nashville, TN; <sup>6</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN

- ThP 421 **Spatial Probabilistic Mapping of Metabolite Ensembles in MALDI Mass Spectrometry Imaging**; Denis Abu Sammour<sup>1, 2</sup>; James L. Cairns<sup>3, 4</sup>; Tobias Boskamp<sup>5, 6</sup>; Christian Marsching<sup>3, 5</sup>; Tobias Kessler<sup>7, 8</sup>; Carina Ramallo Guevara<sup>3</sup>; Verena Panitz<sup>8, 9</sup>; Ahmed Sadik<sup>8, 10</sup>; Jonas Cordes<sup>2, 11</sup>; Stefan Schmidt<sup>3</sup>; Shad A. Mohammed<sup>2, 3</sup>; Miriam F. Rittel<sup>2, 3</sup>; Mirco Friedrich<sup>12, 13</sup>; Michael Platten<sup>12, 13</sup>; Ivo Wolf<sup>2, 11</sup>; Andreas Von Deimling<sup>14</sup>; Christiane A. Opitz<sup>8, 9</sup>; Wolfgang Wick<sup>7, 8</sup>; Carsten Hopf<sup>2, 3, 4</sup>; <sup>1</sup>Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim University of Applied Sciences, Mannheim, Germany; <sup>2</sup>Institute for Medical Technology, Heidelberg University and Mannheim University of Applied Sciences, Mannheim, Germany; <sup>3</sup>Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim University of Applied Sciences, Mannheim, Germany; <sup>4</sup>Medical Faculty Heidelberg, Heidelberg University, Heidelberg, Germany; <sup>5</sup>Bruker Daltonics GmbH & Co.KG, Bremen, Germany; <sup>6</sup>Center for Industrial Mathematics, University of Bremen, Bremen, Germany; <sup>7</sup>Clinical Cooperation Unit Neurooncology, German Cancer Consortium, German Cancer Research Center (DKFZ), Heidelberg, Germany; <sup>8</sup>German Cancer Research Center (DKFZ), Heidelberg, Division of Metabolic Crosstalk in Cancer and the German Cancer Consortium (DKTK), DKFZ Core Center Heidelberg, Heidelberg, Germany; <sup>9</sup>Department of Neurology and National Center for Tumor Diseases, Heidelberg University Hospital, Heidelberg, Germany; <sup>10</sup>Faculty of Bioscience, Heidelberg University, Heidelberg, Germany; <sup>11</sup>Faculty of Computer Science, Mannheim University of Applied Sciences, Mannheim, Germany; <sup>12</sup>Department of Neurology, MCTN, Medical Faculty Mannheim, Heidelberg University, Mannheim, Germany; <sup>13</sup>DKTK Clinical Cooperation Unit Neuroimmunology and Brain Tumor Immunology, DKFZ, Heidelberg, Germany; <sup>14</sup>Department of Neuropathology, University Hospital Heidelberg, and, Clinical Cooperation Unit Neuropathology, German Cancer Research Center (DKFZ), German Cancer Consortium, Heidelberg, Germany

- ThP 422 **Qu-Cee: An Automated Quality Control Pipeline for Cohort and 3-D Imaging Mass Spectrometry**; Lukasz Migas<sup>1</sup>; Ólöf G. Ísberg<sup>2, 3</sup>; David M. G. Anderson<sup>2</sup>; Katerina V Djambazova<sup>2, 3</sup>; Martin Dufresne<sup>2</sup>; Madeline E Colley<sup>2, 4</sup>; Ali Zahraei<sup>2, 3</sup>; Jeffrey M Spraggins<sup>2, 3, 4, 5, 6</sup>; Raf Van De Plas<sup>1, 2, 4</sup>; <sup>1</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>2</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>3</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>4</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>5</sup>Department of Chemistry, Vanderbilt University, Nashville, TN

- ThP 423 **Pyxis Unveiled: Advancing Single-Cell MALDI MSI Analysis for Deeper Molecular Insights**; Ismael Zamora<sup>1</sup>; Rachelle Balez<sup>2</sup>; Jayden C. McKinnon<sup>2</sup>; Reuben S.E. Young<sup>2</sup>; Liam Robinson<sup>2</sup>; Lezanne Ooi<sup>2</sup>; Giuseppe Arturi<sup>3</sup>; Giulia Sorbi<sup>3</sup>; Shane Ellis<sup>2</sup>; Sara Tortorella<sup>3</sup>; <sup>1</sup>Mass Analytica, S.L, Sant Cugat del Vallés, Spain; <sup>2</sup>Molecular Horizons,



## THURSDAY POSTERS

- University of Wollongong, Wollongong, Australia; <sup>3</sup>Mass Analytica, S.L, Bettona, Italy
- ThP 424 **Measuring Metabolic Fluxes Spatially in Tissues by using Mass Spectrometry Imaging;** Kevin Cho<sup>1</sup>; Michaela Schwaiger-Haber<sup>2</sup>; Ethan Stancliffe<sup>2, 3</sup>; Dhanalakshmi S Anbukumar<sup>2</sup>; Kayla Adkins-Travis<sup>2</sup>; Leah P. Shriver<sup>2</sup>; Gary J. Patti<sup>2</sup>; <sup>1</sup>Washington University School of Medicine, St. Louis, MO; <sup>2</sup>Washington University in Saint Louis, St. Louis, MO; <sup>3</sup>Panome Bio, Saint Louis, MO
- ThP 425 **imzML Analyzer - open source Python tool for rapid evaluation of MS imaging data: Application to ecotoxicological model *Dreissena bugensis*;** Matthias Ochs<sup>1</sup>; Nils Weidner<sup>1</sup>; Andreas Roempp<sup>1</sup>; <sup>1</sup>Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany
- ThP 426 **MS Imaging Spectrum Annotation Tool using Accurate Mass and Isotope Pattern Analysis;** Jeff Dahl<sup>1</sup>; Toshiya Matsubara<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD
- ThP 427 **Unsupervised co-registration of H&E microscopic images and mass spectrometry images (MSI) with neural networks;** Sai Srikanth Lakkimsetty; <sup>1</sup>Northeastern University, Boston, MA
- ThP 428 **Assessing Deep Learning Embeddings for MALDI Colocalization;** Lalin Theverapperuma<sup>1</sup>; Leiver Campeon<sup>1</sup>; Nicolas Narvaez Olaya<sup>1</sup>; Pasindu Tennakoon<sup>1</sup>; Andi Krupke<sup>1</sup>; <sup>1</sup>Expert Intelligence, Santa Clara, CA
- ThP 429 **Artificial Intelligence Tools for Comprehensive 3D Molecular Mapping of Microglia in Mouse Brain Using Mass Spectrometry Imaging;** Aditya Kangune<sup>1</sup>; Connor H Beveridge<sup>2</sup>; Matthew Muhoberac<sup>2</sup>; Jason Finley<sup>2</sup>; Jitika Rajpoot<sup>2</sup>; Palak Manchanda<sup>2</sup>; Lixue Jiang<sup>2</sup>; Emerson Hernly<sup>2</sup>; Julia Laskin<sup>2</sup>; Gaurav Chopra<sup>2, 3, 4, 5, 6, 7, 8</sup>; <sup>1</sup>Purdue University, Department of Statistics, West Lafayette, IN; <sup>2</sup>Department of Chemistry, Purdue University, West Lafayette, IN; <sup>3</sup>Department of Computer Science (by courtesy), Purdue University, West Lafayette, IN; <sup>4</sup>Purdue Institute for Drug Discovery, West Lafayette, IN; <sup>5</sup>Regenstrief Center for Healthcare Engineering, West Lafayette, IN; <sup>6</sup>Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; <sup>7</sup>Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; <sup>8</sup>Purdue Institute for Integrative Neuroscience, West Lafayette, IN
- IMAGING MS: DISEASE MARKERS**  
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- ThP 430 **Exploring cutaneous melanoma through spatially-resolved metabolomics via mass spectrometry imaging and machine learning algorithms;** Yu-Hsuan Chen<sup>1</sup>; Laura Min Xuan Chai<sup>1</sup>; Jia-Fang Tsai<sup>2</sup>; Yi-Hua Liao<sup>2</sup>; Cheng-Chih Hsu<sup>1, 3</sup>; <sup>1</sup>Department of Chemistry, National Taiwan University, Taipei, Taiwan; <sup>2</sup>Department of Dermatology, National Taiwan University, Taipei, Taiwan; <sup>3</sup>Leeuwenhoek Laboratories, Co. Ltd., Taipei, Taiwan
- ThP 431 **Spatial mapping of sulfur-containing metabolites in a mouse model of systemic *Staphylococcus aureus* infection;** Justin Ellenburg<sup>1</sup>; Cristina Kraemer-Zimpel<sup>2</sup>; Paige Kies<sup>2</sup>; Neal D Hammer<sup>2</sup>; Boone M. Prentice<sup>1</sup>; <sup>1</sup>University of Florida, GAINESVILLE, FL; <sup>2</sup>Michigan State University, East Lansing, MI
- ThP 432 **MALDI-MSI Visualization of Cardiolipin Alteration in Rat Organ Tissues after Acute and Chronic Oxidative Stress;** Hay-Yan J. Wang<sup>1</sup>; Chih Le Liu<sup>1</sup>; Ping-Ju Tsai<sup>2</sup>; Kuo-Chen Hung<sup>3</sup>; <sup>1</sup>Department of Biological Sciences, National Sun Yat-Sen University, Kaohsiung City, Taiwan; <sup>2</sup>Department of Surgery, Yuan's General Hospital, Kaohsiung City, Taiwan; <sup>3</sup>Division of General and Digestive Surgery, Kaohsiung Medical University Chung-Ho Memorial Hospital, Kaohsiung City, Taiwan
- ThP 433 **Utilizing mass spectrometry imaging to identify potential N-glycan prognostic biomarkers for Temozolomide resistance in Glioblastoma Multiforme tissues;** Aaron Angerstein<sup>1</sup>; Lynsday E.A. Young<sup>1</sup>; Xueqing Lun<sup>2</sup>; Grace Grimsley<sup>1</sup>; Donna L Senger<sup>2, 3, 4, 5</sup>; Sabine Hombach-Klonisch<sup>6, 7</sup>; Thomas Klonisch<sup>6, 7, 8</sup>; Richard R Drake<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC; <sup>2</sup>Arnie Charbonneau Cancer Institute, Cumming School of Medicine, University of Calgary, Calgary, AB; <sup>3</sup>Department of Oncology, Cumming School of Medicine, University of Calgary, Calgary, AB; <sup>4</sup>Gerald Bronfman Department of Oncology, McGill University, Montreal, QC; <sup>5</sup>Lady Davis Institute for Medical Research, Montreal, QC; <sup>6</sup>Human Anatomy and Cell Science, University of Manitoba, Winnipeg, MB; <sup>7</sup>Pathology, University of Manitoba, Rady Faculty of Health Sciences, Max Rady College of Medicine, Winnipeg, MB; <sup>8</sup>CancerCare Manitoba Research Institute, Winnipeg, MB
- ThP 434 **Multimodal MSI and computational analysis of single amyloid beta (A $\beta$ ) plaques reveals A $\beta$  peptide and lipid profiles in Alzheimer's pathology;** Elisabeth Müller<sup>1, 2</sup>; Thomas Enzlein<sup>1</sup>; Carsten Hopf<sup>1, 2</sup>; <sup>1</sup>Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), University of Applied Sciences Mannheim, Mannheim, Germany; <sup>2</sup>Medical Faculty, Heidelberg University, Heidelberg, Germany
- ThP 435 **Metabolic and Lipidomic Alterations in STZ-Induced Diabetic Mouse Kidneys Revealed Using nano-DESI Mass Spectrometry Imaging;** Syeda Nazifa Wali<sup>1</sup>; Manxi Yang<sup>1</sup>; Frederick Nguete Meke<sup>2</sup>; Zhong-Yin Zhang<sup>2</sup>; Julia Laskin<sup>1</sup>; <sup>1</sup>Purdue University, Department of Chemistry, West Lafayette, IN; <sup>2</sup>Purdue University, Department of Medicinal Chemistry and Molecular Pharmacology, West Lafayette, IN
- ThP 436 **Mouse model of breast tumor progression shows specific lipid signals linked to Cyp27b1 ablation in the mammary epithelium;** Mengdi Xing<sup>1</sup>; Ethan Yang<sup>2</sup>; Jiarong Li<sup>1</sup>; Ami Grunbaum<sup>1</sup>; Pierre Chaurand<sup>2</sup>; Richard Kremer<sup>1</sup>; <sup>1</sup>McGill University, Montreal, QC; <sup>2</sup>University of Montreal, Montreal, QC
- ThP 437 **Application of MALDI-MSI to identify and visualize inflammatory mediators in a thermal burn pig skin model;** David Beaver<sup>1</sup>; Celeste C. Finnerty<sup>1</sup>; Andrzej Kudlicki<sup>1</sup>; Brendan Prideaux<sup>1</sup>; <sup>1</sup>University of Texas Medical Branch at Galveston, Galveston, TX
- ThP 438 **Isotope Encoded Spatial Biology identifies Alzheimer Pathology induced Synaptotoxicity in Space and Time;** Jorg Hanrieder; <sup>1</sup>University of Gothenburg, Mölndal, Sweden
- ThP 439 **ToF-SIMS imaging reveals changes in tumor cell lipids during metastatic progression of melanoma;** Noora Neittaanmäki<sup>1</sup>; Oscar Zaar<sup>2</sup>; Kevin Sjögren Cehajic<sup>1</sup>; Kelly Dimovska Nilsson<sup>1</sup>; Dimitrios Katsarelis<sup>2</sup>; Roger Olofsson Bagge<sup>1</sup>; John Paoli<sup>1</sup>; John Fletcher<sup>1</sup>; <sup>1</sup>University of Gothenburg, Gothenburg, Sweden; <sup>2</sup>Sahlgrenska University Hospital, Gothenburg, Sweden
- ThP 440 **Long-Term Lipidomic Changes After Traumatic Brain Injury Using Desorption Electrospray Ionization - Cyclic Ion Mobility Spectrometry - Mass Spectrometry Imaging;** Ludovic Muller<sup>1</sup>; Nivedita Hegdekar<sup>2</sup>; Chinmoy Sarkar<sup>2</sup>; Marta M. Lipinski<sup>2</sup>; Maureen A. Kane<sup>1</sup>; <sup>1</sup>University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD; <sup>2</sup>University of Maryland, School of Medicine, Department of Anesthesiology, Baltimore, MD
- ThP 441 **Analysis of Metabolite Distribution in Rat Liver of High-Fat Model by Mass Spectrometry Imaging;** Hongmei Mao<sup>1</sup>; Wenjun Wang<sup>2</sup>; Xuesong Xiang<sup>1</sup>; Yan Li<sup>1</sup>; Jinpeng Zhao<sup>1</sup>; Yin Huang<sup>3</sup>; Shuangshuang Di<sup>4, 5</sup>; Qin Zhuo<sup>1</sup>; Honggang Nie<sup>4, 5</sup>; <sup>1</sup>Key Laboratory of Trace Element Nutrition of National Health Commission, National Institute for Nutrition and Health, Chinese Center for Diseases Control and Prevention, Beijing, China; <sup>2</sup>Beijing Junfeix Technology Co., Ltd, Beijing, China; <sup>3</sup>Suzhou PANOMIX Biomedical Technology Co., Ltd, Suzhou, China; <sup>4</sup>Beijing National Laboratory for Molecular Sciences, Peking University, Beijing, China; <sup>5</sup>Analytical Instrumentation Center, Peking University, Beijing, China

## THURSDAY POSTERS

- ThP 442 **Dissecting immunometabolism of delta-sarcoglycan deficient hamster model with multimodal mass spectrometry imaging;** Maiko Okamura<sup>1</sup>; Shinichi Yamaguchi<sup>2</sup>; Takushi Yamamoto<sup>2</sup>; Koji Okuda<sup>2</sup>; Shuji Yamashita<sup>3</sup>; Kisasi Amemiya<sup>4</sup>; Kenji Minatoya<sup>5</sup>; Hidetoshi Masumoto<sup>6</sup>; Satoru Noguchi<sup>7</sup>; Ichizo Nishino<sup>8</sup>; Hatsue Ueda<sup>9</sup>; Masaya Ikegawa<sup>3</sup>; <sup>1</sup>Department of Life and Medical Systems, Doshisha University, Kyotanabe-city, Japan; <sup>2</sup>Shimadzu Corporation, Nakagyo-ku, Japan; <sup>3</sup>Doshisha University, Kyotanabe-city, Japan; <sup>4</sup>Department of Pathology, National Cerebral and Cardiovascular Center, Suita-city, Japan; <sup>5</sup>Department of Cardiovascular Surgery, Graduate School of Medicine, Kyoto University, Sakyo-ku, Japan; <sup>6</sup>Graduate School of Medicine, Kyoto University, Sakyo-ku, Japan; <sup>7</sup>Department of Neuromuscular Research, National Center of Neurology and Psychiatry, Kodaira-city, Japan; <sup>8</sup>National Center of Neurology and Psychiatry, Kodaira-city, Japan; <sup>9</sup>National Cerebral and Cardiovascular Center, Suita-city, Japan; <sup>10</sup>Department of Diagnostic Pathology, Hokusetsu General Hospital, Takatsuki-city, Japan
- ThP 453 **MALDI mass spectrometry imaging in oriented *Caenorhabditis elegans* sections;** Ryutaro Jacobson<sup>1</sup>; Elizabeth W. Smith<sup>2</sup>; Yasuaki Saito<sup>1, 3</sup>; Tian Autumn Qiu<sup>1</sup>; <sup>1</sup>Michigan State University Department of Chemistry, East Lansing, MI; <sup>2</sup>Department of Chemistry, Allegheny College, Meadville, PA; <sup>3</sup>School of Pharmacy, Kitasato University, Shirokane, Minato, Japan
- ThP 454 **Comparing three different ways of oocyte washing before MALDI IMS analysis of lipids;** Paulina Kret<sup>1</sup>; Anna Bodzon-Kulakowska<sup>1</sup>; Przemyslaw Mielczarek<sup>1</sup>; Dominika Siekierska<sup>2</sup>; Wieslawa Mlodawska<sup>2</sup>; Piotr Suder<sup>1</sup>; <sup>1</sup>AGH University of Krakow, Kraków, Poland; <sup>2</sup>University of Agriculture, Cracow, Poland
- ThP 455 **A workflow for visualizing and annotating oxidized lipids in mass spectrometry imaging analyses;** Kisurb Choe<sup>1</sup>; Lia Tesfay<sup>2</sup>; Jennifer Kyle<sup>1</sup>; Josie G Eder<sup>1</sup>; Theodore Alexandrov<sup>3</sup>; Maria Fedorova<sup>4</sup>; Suzy Torti<sup>2</sup>; Christopher Robert Anderton<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>University of Connecticut, Storrs, CT; <sup>3</sup>EMBL, Heidelberg, Germany; <sup>4</sup>Dresden University of Technology, Dresden, Germany
- ThP 456 **prmlmaging: an integrated workflow for the analysis and interpretation of spatial on-tissue tandem mass spectrometry of lipids;** Nannan Tao<sup>1</sup>; Bram Heijs<sup>2</sup>; Tobias Boskamp<sup>2</sup>; Soeren-Oliver Deininger<sup>2</sup>; Nikolas Kessler<sup>2</sup>; Arne Fuetterer<sup>2</sup>; Arne Behrens<sup>2</sup>; Corinna Henkel<sup>2</sup>; Nadine T. Smit<sup>2</sup>; Katherine Stumpo<sup>3</sup>; <sup>1</sup>Bruker Daltonics Inc., Billerica, MA; <sup>2</sup>Bruker Daltonics, Bremen, Germany; <sup>3</sup>Bruker Daltonics, Billerica, MA
- ThP 457 **Deep molecular coverage at faster throughput: IR Guided MALDI Imaging in cancer research;** Arne Behrens<sup>1</sup>; Domenic Dreisbach<sup>2</sup>; Ethan Yang<sup>3</sup>; Peng Wang<sup>4</sup>; Annika Nyhuis<sup>1</sup>; Soeren-Oliver Deininger<sup>1</sup>; Joshua L. Fischer<sup>3</sup>; Azad Eshghi<sup>3</sup>; Hans-Christian Koch<sup>2</sup>; <sup>1</sup>Bruker Daltonics GmbH & Co.KG, Bremen, Germany; <sup>2</sup>Bruker Optics GmbH & Co. KG, Ettlingen, Germany; <sup>3</sup>Bruker Scientific, 40 Manning Road, Billerica, MA; <sup>4</sup>Bruker Optics LLC, Billerica, MS
- ThP 458 **Hyperplex MALDI-IHC Proteomics Imaging Reveals the Heterogeneity of Endometrial Cancer Spatial Structure;** Mengze Zhang<sup>1,2</sup>; John Abbey<sup>2,3</sup>; Pierre Bost<sup>4</sup>; Mark J. Lim<sup>5</sup>; Gargey B. Yagnik<sup>5</sup>; Andrew Yatsuhashi<sup>5</sup>; Kenneth J. Rothschild<sup>5, 6, 3</sup>; Bernd Bodenmiller<sup>2, 3</sup>; <sup>1</sup>University of Zurich, Zurich, Switzerland; <sup>2</sup>ETH Zurich, Zurich, Switzerland; <sup>3</sup>University of Zurich, Zürich, Switzerland; <sup>4</sup>Institut Curie, PSL University, Sorbonne Université, Paris, France; <sup>5</sup>AmberGen Inc., Billerica, MA; <sup>6</sup>Boston University, Department of Physics and Photonics Center, Boston, MA
- ThP 459 **Single-cell Multiplexed Imaging and Profiling with Fluorescence-Ion Microscopy (FIM);** Yuchen Xiang<sup>1</sup>; Daniel Simon<sup>1</sup>; Stefania Maneta-Stavarakaki<sup>1</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College London, London, United Kingdom
- ThP 460 **Expansion Imaging Mass Spectrometry for High Spatial Resolution Lipid Analysis using a Superabsorbent Hydrogel;** Jacob M Samuel<sup>1</sup>; Tingting Yan<sup>2</sup>; Boone M. Prentice<sup>2</sup>; <sup>1</sup>University of Florida Department of Chemistry, Gainesville, FL; <sup>2</sup>University of Florida, Chemistry Department, Analytical Chemistry Division, Gainesville, FL
- ThP 461 **Targeted protein imaging of kidney pathologies using MALDI Imaging;** Katherine A. Stumpo<sup>1</sup>; Corinna Henkel<sup>2</sup>; Taylor Skurnac<sup>1</sup>; Jessica Schmitz<sup>3</sup>; Jan Hinrich Braesen<sup>3</sup>; <sup>1</sup>Bruker Scientific, 40 Manning Road, Billerica, MA; <sup>2</sup>Bruker Daltonics GmbH & Co.KG, Bremen, Germany; <sup>3</sup>Nephropathology Unit, Institute for Pathology, Hannover Medical School, Hannover, Germany
- ThP 462 **Light-Activated Derivatization of Lipids for Isomer Analysis by MALDI Mass Spectrometry;** Thomas R Fredriksen<sup>1</sup>; Joseph H Holbrook<sup>2</sup>; Ana L. Mora<sup>3</sup>; Mauricio Rojas<sup>4</sup>; Amanda B Hummon<sup>5, 6</sup>; <sup>1</sup>The Ohio State University, Columbus, OH; <sup>2</sup>The Ohio State Biochemistry Program, Columbus, Ohio; <sup>3</sup>The Ohio State University Department of Internal Medicine Division of Pulmonary, Critical Care & Sleep Medicine, Columbus, Ohio; <sup>4</sup>The Ohio State University
- ThP 443 **Developing an expansion mass spectrometry (ExMS) method to view the (sub)cellular localization of metabolites in single cells;** Jason A Guerrero<sup>1</sup>; Vignesh Venkataramani<sup>2</sup>; Cole Reinholt<sup>2</sup>; Lydia Kisley<sup>2</sup>; Laura M Sanchez<sup>1</sup>; <sup>1</sup>University of California, Santa Cruz, Santa Cruz, CA; <sup>2</sup>Case Western Reserve University, Cleveland, Ohio
- ThP 444 **Utilizing Tandem Repeat Technology for the production of a MALDI-TOF calibration standard with a wide mass coverage;** Jamshid Davoodi; *Biocatalist LLC, Torrance, CA*
- ThP 445 **Oversampling to Achieve Enhanced Spatial Resolution of Zebrafish by Top-Hat IR-MALDESI-MSI;** Alexandria L. Sohn<sup>1</sup>; Morgan M. Ritter<sup>1</sup>; Seth W. Kullman<sup>1</sup>; Andrew P. Bowman<sup>2</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>AbbVie, North Chicago, IL
- ThP 446 **Filter-Assisted Sample Preparation of Liver Organoids for Mass Spectrometry Imaging;** Sohee Yoon<sup>1</sup>; Ahreum Baek<sup>1</sup>; <sup>1</sup>Korea Research Institute of Standards and Science, Daejeon, South Korea
- ThP 447 **Optimization of human eye cryosectioning for biomarker discovery using mass spectrometry imaging;** Junhai Yang<sup>1</sup>; Andrew P. Bowman<sup>1</sup>; Geraint Parfitt<sup>1</sup>; David Wagner<sup>1</sup>; <sup>1</sup>AbbVie, North Chicago, IL
- ThP 448 **Revealing Spatial Proteome on Formalin-Fixed Paraffin-Embedded Tissues via Desorption Electrospray Ionization Mass Spectrometry Imaging Enabled by Integrated Bottom-Up Approach;** Chih-Hsiang Chen<sup>1</sup>; Hsin-Hsiang Chung<sup>1</sup>; Cheng-Chih Hsu<sup>1, 2</sup>; <sup>1</sup>National Taiwan University, Taipei City, Taiwan; <sup>2</sup>Leeuwenhoek Laboratories, Co. Ltd., Taipei, Taiwan
- ThP 449 **Spatiotemporal lipidomic and proteomic landscape of atherosclerotic plaques in hyperlipidemic mice using imaging mass spectrometry;** ROBIN JOSHI<sup>1</sup>; Soon Yew Tang<sup>1</sup>; E. James Petersson<sup>1</sup>; Garret A. FitzGerald<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA
- ThP 450 **Enhancing Tandem Mass Spectrometry Imaging with De-Mosaicking for Multiplexed Lipid Maps on Tissues;** Aolei Tan<sup>1</sup>; Zheng Ouyang<sup>1</sup>; Xiaoxiao Ma<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China
- ThP 451 **Automated on-tissue derivatization for MS imaging with N,N,N-trimethyl-2-(piperazin-1-yl)ethan-1-iodoamine(TMPA) enable us to visualize intrinsic carboxylic acid in murine digestive tract;** Akiko Kubo<sup>1</sup>; Kaoru Nakagawa<sup>2</sup>; Kenta Terashima<sup>2</sup>; Manami Kobayashi<sup>2</sup>; <sup>1</sup>Kobe University, Kobe, Japan; <sup>2</sup>Shimadzu Corporation, Nakagyo-ku, Japan
- ThP 452 **Desium: Spatial Transcriptomics and Metabolomics on Single Human Cancer Tissue Sections with DESI-MSI and Visium Spatial Transcriptomics;** Trevor M. Godfrey<sup>1</sup>; Yasmin Shanneik<sup>1</sup>; Faith Jackobs<sup>1</sup>; Livia S. Eberlin<sup>1</sup>; <sup>1</sup>Baylor College of Medicine, Houston, TX

## THURSDAY POSTERS

- Department of Internal Medicine, Columbus, Ohio; <sup>5</sup>The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio; <sup>6</sup>Comprehensive Cancer Center, The Ohio State University, Columbus, OH, 43210
- ThP 463 **Addition of Heavy Metal Detection to the MALDI IMS Repertoire for Simultaneous Imaging of Exogenous Metals and Endogenous Bioanalytes**; Kes A Luchini<sup>1</sup>; Tara Harvey<sup>2, 3</sup>; Grace M. Thornhill<sup>2, 3</sup>; Abigale S Mikolitis<sup>2, 3</sup>; Zachary J. Sasiene<sup>2, 3</sup>; Joshua D. Breidenbach<sup>2, 3</sup>; Ethan M. McBride<sup>2, 3</sup>; Brett R. Blackwell<sup>2, 3</sup>; Austin R. Anderson<sup>2, 3</sup>; Lauren K. Heine<sup>2, 3</sup>; Chi-Yen Tseng<sup>2, 3</sup>; Jessica A. Salguero<sup>2, 3</sup>; Francisca E. Rodriguez<sup>2, 3</sup>; Salvator J. Palmisano<sup>2, 3</sup>; Erick S. LeBrun<sup>2, 3</sup>; Phillip M. Mach<sup>2, 3</sup>; Trevor G. Glaros<sup>2, 3</sup>; Emilio S. Rivera<sup>2, 3</sup>; <sup>1</sup>Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>3</sup>Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM
- ThP 464 **Cellular-level resolution DESI-MS imaging**; Chengyi XIE<sup>1, 2</sup>; Jianing WANG<sup>1, 2</sup>; Zongwei CAI<sup>1, 2</sup>; <sup>1</sup>State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Kowloon Tong, Kowloon, China; <sup>2</sup>Department of Chemistry, Hong Kong Baptist University, Kowloon Tong, Kowloon, China
- ThP 465 **Submicron Resolution MALDI Mass Spectrometry Imaging of Lipids at the Subcellular Level**; Chengyi Xie<sup>1, 2</sup>; Jianing Wang<sup>1</sup>; Zongwei Cai<sup>1, 2</sup>; <sup>1</sup>State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, China; <sup>2</sup>Department of Chemistry, Hong Kong Baptist University, Kowloon Tong, Kowloon, China
- ThP 466 **Molecular profiling of glioblastoma patient-derived single cells using combined MSI and MALDI-IHC**; Kasper K Krestensen<sup>1</sup>; Marleen Derwede<sup>2</sup>; Frederik De Smet<sup>2</sup>; Eva Cuyper<sup>1</sup>; Ron Heeren<sup>1</sup>; <sup>1</sup>M&I Division of Imaging Mass Spectrometry, Maastricht University, Maastricht, Netherlands; <sup>2</sup>KU Leuven, Leuven, Belgium
- ThP 467 **Met-ID: a graphical user interface for rapid MALDI-MSI metabolite identification**; Patrik Bjärterot<sup>1</sup>; Anna Nilsson<sup>1</sup>; Reza Shariatgorji<sup>1</sup>; Theodosia Vallianatou<sup>1</sup>; Ibrahim Kaya<sup>1</sup>; Lukas Käll<sup>2</sup>; Per Svenningsson<sup>3</sup>; Per E. Andrén<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>Royal institute of Technology, Stockholm, Sweden; <sup>3</sup>Karolinska Institutet, Stockholm, Sweden
- ThP 468 **Imaging Technologies for Constructing 3D Multimodal Lipid Atlases of the Eye**; David M. G. Anderson<sup>1</sup>; Lukasz Migas<sup>2</sup>; Jeffery Messinger<sup>3</sup>; Raf Van De Plas<sup>2</sup>; Dongfeng N Cao<sup>4</sup>; Richard M. Caprioli<sup>1</sup>; Christine A Curcio<sup>3</sup>; Kevin L. Schey<sup>1</sup>; Jeffrey M Spraggins<sup>5</sup>; <sup>1</sup>Vanderbilt University, Department of Biochemistry, Nashville, TN; <sup>2</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>3</sup>University of Alabama Birmingham, Birmingham, Alabama; <sup>4</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>5</sup>Vanderbilt University, Nashville, TN
- ThP 469 **Uncovering ferroptotic cells as pathogenic drivers in diseased tissue using Dual-SIMS imaging at 1 µm resolution**; Hua Tian<sup>1</sup>; Kavita Vats<sup>2</sup>; Louis J. Sparvero<sup>1</sup>; Kunal Singh<sup>2</sup>; Yulia Y. Tyurina<sup>1</sup>; Hülya Bayır<sup>3</sup>; Valeria E. Kagan<sup>1</sup>; Yuri L. Bunimovich<sup>2</sup>; <sup>1</sup>Center for Free Radical and Antioxidant Health, Department of Environmental Health and Occupational Health, University of Pittsburgh, Pittsburgh, PA; <sup>2</sup>Department of Dermatology, University of Pittsburgh School of Medicine, Pittsburgh, PA; <sup>3</sup>Department of Pediatrics, Division of Critical Care and Hospital Medicine, Redox Health Center, Vagelos College of Physicians and Surgeons, Columbia University Irving Medical Center, New York, NY
- ThP 470 **Enhancing MALDI IMS Sensitivity and Specificity of Neutral Lipids via Salt Doping and Ion Mobility**; Kameron Molloy<sup>1, 2</sup>; Madeline E Colley<sup>2, 3</sup>; Martin Dufresne<sup>2, 3</sup>; Lukasz Migas<sup>2, 4</sup>; Raf Van De Plas<sup>2, 3, 4</sup>; Jeffrey M Spraggins<sup>1, 2, 3, 5, 6</sup>; <sup>1</sup>Department of Chemistry, Vanderbilt University, Nashville, TN; <sup>2</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>3</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>4</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>5</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>6</sup>Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN
- ThP 471 **MALDI-2 Mass Spectrometry Imaging of Peptide Toxins, Lipopeptides and Lipids in Thin Sections of Bacillus subtilis Biofilms**; Kim Lena Wüpping<sup>1</sup>; Jan-Philipp Knepper<sup>1</sup>; Alexander Potthoff<sup>1</sup>; Jens Soltwisch<sup>1</sup>; Klaus Dreisewerd<sup>1</sup>; <sup>1</sup>Institute of Hygiene, University of Münster, Münster, Germany
- ThP 472 **Image Deconvolution Restores MSI Spatial Resolution Following Signal Averaging**; Yury Desyaterik<sup>1</sup>; Mary Peace McRae<sup>2</sup>; Angela DM Kashuba<sup>1</sup>; Konstantin O. Nagornov<sup>3</sup>; Anton N. Kozhinov<sup>3</sup>; Yury O. Tsybin<sup>3</sup>; Elias P. Rosen<sup>1</sup>; <sup>1</sup>UNC, Chapel Hill, NC; <sup>2</sup>University of Virginia, Charlottesville, VA; <sup>3</sup>Spectroswiss, Lausanne, Switzerland
- ThP 473 **Lithium doped nanospray desorption electrospray ionization mass spectrometry imaging for enhanced metabolite coverage**; Kiera Nguyen<sup>1</sup>; Nathalie Costie<sup>2</sup>; Gillian Carleton<sup>2, 3</sup>; Tian Zhao<sup>2, 3</sup>; Julian J. Lum<sup>2, 3</sup>; Kyle D Duncan<sup>1, 4</sup>; <sup>1</sup>Department of Chemistry, Vancouver Island University, Nanaimo, BC; <sup>2</sup>Trev and Joyce Deeley Research Centre, BC Cancer, Victoria, BC; <sup>3</sup>Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; <sup>4</sup>Department of chemistry, University of Victoria, Victoria, BC
- ThP 474 **MS imaging enabling visualization of lipid C=C positional isomers in biological tissues using Oxygen Attachment Dissociation (OAD)**; Kaoru Nakagawa<sup>1</sup>; Hidenori Takahashi<sup>1</sup>; Satoshi Kasamatsu<sup>1</sup>; Kengo Takeshita<sup>1</sup>; Manami Kobayashi<sup>2</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>SHIMADZU Corporation, Kawasaki, Japan
- ThP 475 **New workflows for 3-D multimodal molecular imaging based on sequential 2-D data**; Ellie L Pingry<sup>1, 2</sup>; Lukasz Migas<sup>3, 4</sup>; David Anderson<sup>1, 5</sup>; Felipe A Moser<sup>4</sup>; Angela R. S. Kruse<sup>1, 2</sup>; Melissa A. Farrow<sup>3, 5</sup>; Raf Van De Plas<sup>1, 4, 5</sup>; Jeffrey M Spraggins<sup>1, 2, 5, 6, 7</sup>; <sup>1</sup>Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; <sup>2</sup>Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; <sup>3</sup>Mass Spectrometry Research Center, Nashville, TN; <sup>4</sup>Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; <sup>5</sup>Department of Biochemistry, Vanderbilt University, Nashville, TN; <sup>6</sup>Department of Chemistry, Vanderbilt University, Nashville, TN; <sup>7</sup>Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN
- ThP 476 **Advances in top-down HRMS with AP/MALDI orbitraps for spatial analysis of peptides/metabolites in human pathology FFPE tissue archives**; Peter D. Verhaert<sup>1</sup>; Gilles Frache<sup>2</sup>; Maureen Feucherolles<sup>2</sup>; Sooraj Baijnath<sup>3</sup>; Aletta Millen<sup>3</sup>; Dick Swaab<sup>4, 5</sup>; Lin Zhang<sup>4</sup>; Cecilia Lindskog<sup>6</sup>; Mathias Uhlén<sup>6</sup>; Marthe Verhaert<sup>7</sup>; Raf Sciort<sup>8</sup>; <sup>1</sup>ProteoFormIX, Beerse, Belgium; <sup>2</sup>Luxembourg Institute of Science and Technology, Belvaux, Luxembourg; <sup>3</sup>Integrated Molecular Physiology Research Initiative, Johannesburg, South Africa; <sup>4</sup>Netherlands Institute for Neuroscience, Amsterdam, Netherlands; <sup>5</sup>Uppsala university, Uppsala, Sweden; <sup>6</sup>KTH Royal Institute of Technology, Stockholm, Sweden; <sup>7</sup>BITOX Belgian Immunotoxicity Board, Brussels, Belgium; <sup>8</sup>University Hospitals Leuven, Heverlee, Belgium

### INFORMATICS: GENERAL, SRM, AND DIA 477-484

- ThP 477 **DeepRTAlign: toward accurate retention time alignment for large cohort mass spectrometry data analysis**; Yi Liu; Beijing Proteome Research Center, Beijing, China
- ThP 478 **Using Graphs to Visualize and Simplify Complex Mass Spectra**; Ron Bonner<sup>1</sup>; Gerard Hopfgartner<sup>2</sup>; <sup>1</sup>Ron Bonner

## THURSDAY POSTERS

- Consulting, Newmarket, ON; <sup>2</sup>University of Geneva, Geneva, Switzerland
- ThP 479 **PepQuery-DIA: Streamlining Fast and Accurate Proteomic Validation of Novel Genomic Alterations Using DIA Data**; Wenrong Chen<sup>1,2</sup>; Matthew V. Holt<sup>1,2</sup>; Yu Wen<sup>3</sup>; Jixin Wang<sup>4</sup>; Wenyan Zhong<sup>5</sup>; Bing Zhang<sup>6</sup>; <sup>1</sup>Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; <sup>2</sup>Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX; <sup>3</sup>Data Science and AI, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD; <sup>4</sup>Oncology Data Science, AstraZeneca, Gaithersburg, MD; <sup>5</sup>Oncology Data Science, Oncology R&D, AstraZeneca, New York, NY; <sup>6</sup>Baylor College of Medicine, Houston, Texas
- ThP 480 **Developing a massive multi-instrument manually curated chromatogram training library**; Brian C. Searle<sup>1</sup>; Ariana E Shannon<sup>1</sup>; Katelyn B Brusach<sup>1</sup>; Regina M Edgington<sup>1</sup>; Gautam Ghosh<sup>1</sup>; Alex W Joyce<sup>1</sup>; Madalyn G Moore<sup>1</sup>; Chase Renzelmann<sup>1</sup>; Damien B Wilburn<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH
- ThP 481 **Automated Quality Control Assessment for Large-Scale Proteomics Datasets**; Niveda Sundararaman<sup>1</sup>; Manasa Vegesna<sup>1</sup>; Aleksandra Binek<sup>1</sup>; Jennifer E. Van Eyk<sup>1</sup>; <sup>1</sup>Cedars Sinai Medical Center, Los Angeles, CA
- ThP 482 **Mass++ ver.4 Gold (official release), an Open-Source MS Data Viewer**; Satoshi Tanaka<sup>1,2</sup>; Masaki Murase<sup>2</sup>; Masaki Kato<sup>2,3</sup>; Hiroyuki Yamamoto<sup>2,4</sup>; Tsuyoshi Tabata<sup>2,5</sup>; Maiko Kusano<sup>2,6</sup>; Shin Kawano<sup>2,7</sup>; Shujiro Okuda<sup>8</sup>; Akiyasu C. Yoshizawa<sup>2,8</sup>; <sup>1</sup>Trans-IT, Mibu-machi, Japan; <sup>2</sup>Mass++ Users Group., Kyoto, Japan; <sup>3</sup>Data Knowledge Organization Unit, RIKEN Information R&D and Strategy Headquarters, RIKEN, Wako, Japan; <sup>4</sup>Human Metabolome Technologies, Inc., Tsuruoka, Japan; <sup>5</sup>Grad. School of Pharma. Sci., Kyoto Univ., Kyoto, Japan; <sup>6</sup>School of Medicine, Showa Univ., Shinagawa, Japan; <sup>7</sup>School of Frontier Engineering, Kitasato Univ., Sagamihara, Japan; <sup>8</sup>Medical AI Center, School of Medicine, Niigata Univ., Niigata, Japan
- ThP 483 **Speeding up panel development for targeted proteomics using deep learning: a proof-of-concept based on a prostate cancer study**; Tikira Temu<sup>1</sup>; Oliver M. Bernhardt<sup>1</sup>; Véronique Laforte<sup>1</sup>; Sebastian Mueller<sup>1</sup>; Tejas Gandhi<sup>1</sup>; Lukas Reiter<sup>1</sup>; <sup>1</sup>Biognosys AG, Schlieren, Switzerland
- ThP 484 **Improved library free dia-PASEF based quantitative proteomics using Spectronaut**; Tejas Gandhi<sup>1</sup>; Monika Pepelnjak<sup>1</sup>; Christopher Below<sup>1</sup>; An-phi Nguyen<sup>1</sup>; Véronique Laforte<sup>1</sup>; Roland Bruderer<sup>1</sup>; Oliver M. Bernhardt<sup>1</sup>; Lukas Reiter<sup>1</sup>; <sup>1</sup>Biognosys AG, Schlieren, Switzerland
- INFORMATICS: MULTOMIC INTEGRATION**  
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- ThP 485 **Nonlinear Dynamic Changes During Human Aging Revealed in Multi-omics Profiles**; Xiaotao Shen<sup>1</sup>; Chuchu Wang<sup>1</sup>; Xin Zhou<sup>1</sup>; Wenyu Zhou<sup>1</sup>; Daniel Hornburg<sup>1</sup>; Si Wu<sup>1</sup>; Michael Snyder<sup>1</sup>; <sup>1</sup>Stanford University, Palo Alto, CA
- ThP 486 **GlycoLibraries: Hybrid-search-based bootstrapping method identifies and annotates oligosaccharides, gangliosides and glycopeptides in complex matrices**; Concepcion Remoroza<sup>1</sup>; Yi Liu<sup>1</sup>; Meghan Burke<sup>1</sup>; Yuxue Liang<sup>1</sup>; Xiaoyu Yang<sup>1</sup>; Tytus Mak<sup>1</sup>; Sergey Sheetlin<sup>1</sup>; Yuri Mirokhin<sup>1</sup>; Dmitrii Tchekhovskoi<sup>1</sup>; Stephen Stein<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology, Gaithersburg, MD
- ThP 487 **Protein profiling of zebrafish embryos unmasks a new regulatory layer during early embryogenesis**; Gabriel Da Silva Pescador<sup>1</sup>; Danielson Baia Amaral<sup>1</sup>; Joseph M Varberg<sup>1</sup>; Ying Zhang<sup>1</sup>; Yan Hao<sup>1</sup>; Laurence Florens<sup>1</sup>; Ariel A Bazzini<sup>1,2</sup>; <sup>1</sup>Stowers Institute for Medical Research, Kansas City, MO; <sup>2</sup>Department of Molecular and Integrative Physiology, University of Kansas School of Medicine, Lawrence, KS
- ThP 488 **Multi-Omics unveils disruption of shared metabolic pathways in Caco-2 Cells and C. elegans exposed to Organophosphate flame retardants.**; Ahn Jeongjun<sup>1</sup>; Kim Hyung Min<sup>2</sup>; Kang Jong Seong<sup>2</sup>; <sup>1</sup>chungnam national university, daejeon, South Korea; <sup>2</sup>Chungnam National University, Daejeon, South Korea
- ThP 489 **Functional Integrative Enrichment Metric Score for proteomics enrichment analysis**; Maciej Dulewicz<sup>1</sup>; Henrik Zetterberg<sup>1,2</sup>; Kaj Blennow<sup>1</sup>; Jörg Hanrieder<sup>1,2</sup>; <sup>1</sup>University of Gothenburg, Gothenburg, Sweden; <sup>2</sup>Department of Neurodegenerative Disease, UCL Institute of Neurology, London, United Kingdom
- ThP 490 **Proteomic Insights into the Effects of Blueberry and Cranberry Crops on Honey Bee Health and Physiology**; Huan Zhong<sup>1</sup>; Yuming Shi<sup>1</sup>; Jason Rogalski<sup>1</sup>; Renata Moravcova<sup>1</sup>; Leonard Foster<sup>1</sup>; <sup>1</sup>UBC, Vancouver, BC
- ThP 491 **Multi-omics characterization of anti-CD40 induced mouse colitis model**; Liang Jin<sup>1</sup>; Michael Macoritto<sup>1</sup>; Nikolaus Berndt<sup>2</sup>; Xue Wang<sup>1</sup>; Ruoqi Peng<sup>1</sup>; Annette Schwartz Serman<sup>1</sup>; Yu Tian<sup>1</sup>; <sup>1</sup>AbbVie Bioresearch Center, Worcester; <sup>2</sup>Doppelganger Biosystem GmbH, Oldenbourg, Germany
- ThP 492 **A multi-scale map of proteome organization from integration of protein interactions and images**; Leah V Schaffer<sup>1</sup>; Mengzhou Hu<sup>1</sup>; Edward L Hutlin<sup>2</sup>; Gege Qian<sup>1</sup>; Abantika Pal<sup>3</sup>; Neelesh Soni<sup>3</sup>; Andrew P Latham<sup>3</sup>; Kyung-Mee Moon<sup>4</sup>; Laura Pontano Vaites<sup>2</sup>; Trang Le<sup>5</sup>; Yue Qin<sup>1</sup>; Dexter Pratt<sup>1</sup>; Christopher Churas<sup>1</sup>; Leonard J Foster<sup>4</sup>; Ignacia Echeverria<sup>3</sup>; J Wade Harper<sup>2</sup>; Steven P. Gygi<sup>2</sup>; Emma Lundberg<sup>5,6,7</sup>; Trey Ideker<sup>1</sup>; <sup>1</sup>University of California, San Diego, San Diego, CA; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>University of California-San Francisco, San Francisco, CA; <sup>4</sup>University of British Columbia, Vancouver, BC; <sup>5</sup>Stanford University, Stanford, CA; <sup>6</sup>KTH Royal Institute of Technology, Stockholm, Sweden; <sup>7</sup>Chan-Zuckerburg Biohub, San Francisco, California
- ThP 493 **M2IA: metabolic pathway-reaction-metabolite-based strategy for advanced integrative analysis of gut microbiome, metabolome, and phenotype**; Yan Ni<sup>1</sup>; Cuifang Xu<sup>1</sup>; <sup>1</sup>Children's Hospital, Zhejiang University School of Medicine, National Clinical Research Center for Child Health, Hangzhou, China
- ThP 494 **Complete, Precise and Fast Proteogenomic Analysis with pAnno2**; Kaifei Wang<sup>1</sup>; Mingkun Yang<sup>2,3</sup>; Zhuohong Wei<sup>1</sup>; Feng Ge<sup>2,3</sup>; Hao Chi<sup>1</sup>; <sup>1</sup>Key Laboratory of Intelligent Information Processing of Chinese Academy of Sciences (CAS), Institute of Computing Technology, Beijing, China; <sup>2</sup>State Key Laboratory of Freshwater Ecology and Biotechnology, Institute of Hydrobiology, Chinese Academy of Sciences, Wuhan, China; <sup>3</sup>Key Laboratory of Algal Biology, Institute of Hydrobiology, Chinese Academy of Sciences, Wuhan, China
- ThP 495 **Integrated Metabolomics and Proteomics Reveals Systemic and Localized Metabolic Disruptions in Colorectal Cancer**; Ethan Stancliffe<sup>1</sup>; Adam D. Richardson<sup>1</sup>; Monil Gandhi<sup>1</sup>; Ashima Mehta<sup>1</sup>; Kevin Y Cho<sup>2</sup>; Gary J. Patti<sup>1,2</sup>; <sup>1</sup>Panome Bio, Saint Louis, MO; <sup>2</sup>Washington University in Saint Louis, St. Louis, MO
- ThP 496 **ShowMEPATH: Automated Multi-Omics Comparative Analysis Tool Unveiling Hidden Patterns in Large-Scale Fold Change Data**; Manhoi Hur<sup>1,2</sup>; Hee-Seung Choi<sup>1</sup>; Wilhelmina Van De Ven<sup>1</sup>; Katayoon Dehesh<sup>1</sup>; <sup>1</sup>University of California, Riverside, RIVERSIDE, California; <sup>2</sup>UCR Metabolomics Core, University of California, Riverside, California
- ThP 497 **A systems-scale approach to identifying protein isoforms modulating endothelial cell development**; Madison M Mehler<sup>1</sup>; David Wissel<sup>2</sup>; Erin D Jeffery<sup>1</sup>; Vasilii Pavelko<sup>1</sup>; Jennifer A Korchak<sup>1</sup>; Micah Lehe<sup>1</sup>; Marcus J. Meade<sup>1</sup>; Gloria Sheynkman<sup>1</sup>; <sup>1</sup>University of Virginia, Charlottesville, VA; <sup>2</sup>University of Zurich, Zürich, Switzerland
- ThP 498 **Deep plasma proteomics enables identification of sample-swap issues in a large multi-omics discovery study**; Yuntao Hu<sup>1</sup>; Jinlyung Choi<sup>1</sup>; Ajinkya Kokate<sup>1</sup>; Sara Nouri Golmaei<sup>1</sup>; Daniel Ariad<sup>1</sup>; Ehdieh Khaledian<sup>1</sup>; Guanhua Shu<sup>1</sup>; Purva Ranjan<sup>1</sup>; Manway Liu<sup>1</sup>; Joon-Yong Lee<sup>1</sup>; Bruce

## THURSDAY POSTERS

- Wilcox<sup>1</sup>; Chinmay Belthangady<sup>1</sup>; <sup>1</sup>Prognomiq Inc., San Mateo, California
- ThP 499 **Unique opportunities in cross-omics analysis of plasma multiomics data using prior knowledge**; Austin Quach<sup>1,2</sup>; Whitaker Cohn<sup>2</sup>; Rachel Kwan<sup>1</sup>; Olivia Choi<sup>1</sup>; Seungjun Yeo<sup>1</sup>; Julian Whitelegge<sup>2</sup>; <sup>1</sup>Dalton Bioanalytics Inc., Los Angeles, CA; <sup>2</sup>UCLA Pasarow Mass Spectrometry Laboratory, Los Angeles, CA
- ThP 500 **Proteomager: an integrative platform for image coregistration, spatial analysis, and visualization for high-resolution spatial proteomics datasets**; Zhenru Zhou<sup>1</sup>; Amanda Lorentzian<sup>1</sup>; Yikai Luo<sup>1</sup>; Zhichang Yang<sup>1</sup>; Anatoly Belov<sup>1</sup>; Melissa Gonzalez<sup>1</sup>; Miriam Baca<sup>1</sup>; James Ziai<sup>1</sup>; Ying Zhu<sup>1</sup>; Meena Choi<sup>1</sup>; <sup>1</sup>Genentech Inc., South San Francisco, CA
- ThP 501 **Integration of untargeted metabolomics with targeted profiling of inflammatory proteins to define the metabolic fingerprint of inflammation in COVID-19**; Monil Gandhi<sup>1</sup>; Adam Richardson<sup>2</sup>; Ethan Stancliffe<sup>2</sup>; Ashima Mehta<sup>2</sup>; Kevin Y Cho<sup>3</sup>; Gary J. Patti<sup>1,3</sup>; <sup>1</sup>PanomeBio, St Louis, MO; <sup>2</sup>Panome Bio, St Louis, MO; <sup>3</sup>Washington University in Saint Louis, St. Louis, MO
- ThP 502 **SimpliFi in a Box: multiomics data analysis on private servers**; Jim Palmeri<sup>1</sup>; John P Wilson<sup>1</sup>; <sup>1</sup>Protifi, LLC, Fairport, NY
- INSTRUMENTATION: NEW CONCEPTS**  
503-519
- ThP 503 **Comparison of Laser-induced Acoustic Desorption/Molecular Rotational Resonance (LIAD/MRR) Spectroscopy to GCxGC/EI MS as a Structure Elucidation Method**; Caroline E. R. Rowell<sup>1</sup>; Jaskiran Kaur<sup>1</sup>; Ruth O. Anyaeche<sup>1</sup>; Yuyang Zhang<sup>1</sup>; Kawthar Z. Alzarani<sup>1,2</sup>; Hendrik M. Ma<sup>1</sup>; Annika M. Little<sup>1</sup>; Tanya Sharma<sup>1</sup>; Matthan D. Nussbaum<sup>1</sup>; Drake A. Hershberger<sup>1</sup>; Ying-jou Lee<sup>1</sup>; Voislav Blagojevic<sup>3</sup>; Justin L. Neill<sup>3</sup>; Hilka I Kenttämää<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Jordan University of Science and Technology, Irbid, Jordan; <sup>3</sup>BrightSpec Inc., Charlottesville, VA
- ThP 504 **Image-Guided Laser Ablation System for Precise 3D Tissue Sampling for Subsequent Analysis of Biomolecules in Cancer Research**; Jan Hahn<sup>1, 2, 3</sup>; Manuela Moritz<sup>1</sup>; Anton Walter<sup>1</sup>; Tamara Wieck<sup>1</sup>; Ayham Moustafa<sup>1</sup>; Marie-Therese Haider<sup>1, 3</sup>; Tobias Lange<sup>1, 4</sup>; Hartmut Schlüter<sup>1, 3</sup>; <sup>1</sup>University Medical Center Hamburg-Eppendorf (UKE), Hamburg, Germany; <sup>2</sup>Mildred Scheel Cancer Career Center HaTriCS4, Hamburg, Germany; <sup>3</sup>University Cancer Center Hamburg, Hamburg, Germany; <sup>4</sup>University Hospital Jena, Jena, Germany
- ThP 505 **Mass Resolution in PTR-TOFMS: The more, the better?**; Alfons Jordan<sup>1</sup>; Christian Lindinger<sup>1</sup>; Andreas Mauracher<sup>1</sup>; Rene Gutmann<sup>1</sup>; Stefan Feil<sup>1</sup>; Paul Mutschlechner<sup>1</sup>; Todd Rogers<sup>2</sup>; Philipp Sulzer<sup>1</sup>; <sup>1</sup>IONICON Analytik GmbH, Innsbruck, Austria; <sup>2</sup>Trace VOC, Kennewick, WA
- ThP 506 **A novel technology for sample preparation: A fully automated, high-throughput and online electro-extraction platform hyphenated to LC-MS analysis**; Yupeng He<sup>1</sup>; Paul Miggiels<sup>1</sup>; Nicolas Drouin<sup>1</sup>; Amy C. Harms<sup>1</sup>; Bert Wouters<sup>1</sup>; Thomas Hankemeier<sup>1</sup>; <sup>1</sup>Leiden University, Leiden, Netherlands
- ThP 507 **Utilizing Charged Residue Mechanism in Electrospray Droplets for Cryo-EM Sample Preparation**; Liwen Liang<sup>1</sup>; Jingjin Fan<sup>1, 2</sup>; Zi Yang<sup>1</sup>; Zheng Pang<sup>1</sup>; Zheng Ouyang<sup>1</sup>; Hong-Wei Wang<sup>1</sup>; Xiaoyu Zhou<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>University of Oxford, Oxford, United Kingdom
- ThP 508 **Mobility Selective Ion Soft-Landing Using Structures for Lossless Ion Manipulation (SLIM)**; Sandilya Garimella<sup>1</sup>; Jung Yun Lee<sup>1</sup>; Ailin Li<sup>1</sup>; Prabhakaran Venkateshkumar<sup>1</sup>; Xin Zhang<sup>1</sup>; Harrilal P Christopher<sup>1</sup>; Libor Kovarik<sup>1</sup>; Yehia M Ibrahim<sup>1</sup>; Richard D Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- ThP 509 **A universal design for high-resolution linear time-of-flight mass spectrometers with a wide m/z range**; Yi-Hong Cai<sup>1</sup>; Yi-Sheng Wang<sup>1</sup>; <sup>1</sup>Genomics Research Center Academia Sinica, Taipei, Taiwan
- ThP 510 **A Functionalized Vacuum Flange to Power Ion Guides, Funnels, and Traps**; Caraleigh G. Smith<sup>1</sup>; Brian H Clowers<sup>2</sup>; Zackary R Kinlein<sup>2</sup>; Steven J Kregel<sup>1</sup>; <sup>1</sup>Bradley University, Peoria, IL; <sup>2</sup>Washington State University Department of Chemistry, Pullman, WA
- ThP 511 **Exploring sex differences in zebrafish livers using a novel targeted discovery metabolomics approach**; Michaela Schwaiger-Haber<sup>1</sup>; Bashar Amer<sup>2</sup>; Darshak Gadara<sup>1</sup>; Cristina C. Jacob<sup>2</sup>; Philip M. Remes<sup>2</sup>; Susan S. Bird<sup>2</sup>; Gary J. Patti<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 512 **Design and optimization of a band-pass device for a quadrupole ion guide**; Yang Kang<sup>1</sup>; Mircea Guna<sup>1</sup>; David Cox<sup>1</sup>; Andrei Sonoc<sup>1</sup>; Ian Moore<sup>1</sup>; Bradley Schneider<sup>1</sup>; <sup>1</sup>SCIEX, Concord, ON
- ThP 513 **Analysis of VOCs in aqueous solutions using the coupling of an oven with a mobile FT-ICR-MS associated to chemical ionization**; Taous ABAR<sup>1</sup>; Michel Heninger<sup>1</sup>; Joel Lemaire<sup>1</sup>; Hélène Mestdagh<sup>1</sup>; <sup>1</sup>Institut de Chimie Physique - Université Paris-Saclay, Orsay, France
- ThP 514 **Streamlining effective translational research using a novel hybrid nominal mass spectrometer acquisition for comprehensive molecular profiling**; Scott Peterman<sup>1</sup>; Scott D Stanley<sup>2</sup>; Abigail Burrows Franco<sup>2</sup>; Phillip Remes<sup>3</sup>; Cristina Jacobs<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Fort Walton Beach, FL; <sup>2</sup>University of Kentucky, Lexington, KY; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 515 **Transmission Nano-Projectile Secondary Ion Mass Spectrometry - A Method for Accurate Analysis of Nanoparticles**; Michael A. Shaw<sup>1</sup>; Michael J. Eller<sup>1</sup>; <sup>1</sup>California State University Northridge, Northridge, CA
- ThP 516 **Virtual-Slit Cycloidal Mass Spectrometry of Actinide Particles**; Rafael Bento Serpa<sup>1</sup>; Charles B. Parker<sup>1</sup>; Elizabeth D. LaBone<sup>2</sup>; Christopher Zarzana<sup>3</sup>; Justin Keogh<sup>4</sup>; Jonathon Andrus<sup>3</sup>; Nathan A. Stevens<sup>3</sup>; Rosalie Greer<sup>2</sup>; Kyle M. Samperton<sup>2</sup>; Danielle Mannion<sup>2</sup>; Joe Mannion<sup>2</sup>; Jeffrey T. Glass<sup>1</sup>; M. Bonner Denton<sup>4</sup>; Jason J. Amsden<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC; <sup>2</sup>Savannah River National Laboratory, Aiken, SC; <sup>3</sup>Idaho National Laboratory, Idaho Falls, ID; <sup>4</sup>University of Arizona, Tucson, AZ
- ThP 517 **Narrowed isolation in the low mass range using a digital QTOF**; Elizabeth Groetsema<sup>1</sup>; Sumeet S. Chakravorty<sup>1</sup>; Fatima Olayemi Obe<sup>1</sup>; Gordon A Anderson<sup>2</sup>; Shane Tichy<sup>3</sup>; Adam P. Huntley<sup>1</sup>; Brian H Clowers<sup>1</sup>; Peter T. A. Reilly<sup>1</sup>; <sup>1</sup>Washington State University Department of Chemistry, Pullman, WA; <sup>2</sup>GAA Custom Electronics LLC, Kennewick, WA; <sup>3</sup>Agilent Technologies, Santa Clara, CA
- ThP 518 **Practical Quadrupole Theory: Rectilinear Quadrupole and Hexapole Ion Guides Operated with Collisional Damping Pressures**; Jacob Pasko<sup>1</sup>; Randall E Pedder<sup>1</sup>; Luke Metzler<sup>1</sup>; <sup>1</sup>Ardara Technologies, Ardara, PA
- ThP 519 **High Dynamic Range Data Acquisition System for TOFMS tools**; Amit Weingarten<sup>1</sup>; Pierre-François Maistre<sup>2</sup>; Aleksey Vorobyev<sup>3</sup>; Vasily Makarov<sup>3</sup>; Anatoly Verenchikov<sup>3</sup>; <sup>1</sup>El-Mul Technologies, Rehovot, Israel; <sup>2</sup>Acqiris SA, Geneva, Switzerland; <sup>3</sup>MSC-CG, Bar, Montenegro
- INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING**  
520-538
- ThP 520 **Evaluation of Gas dynamics of source nozzle geometry by simulation and LDTD-MS/MS experiment**; Pierre Picard<sup>1</sup>; Sarah Demers<sup>1</sup>; Jean Lacoursière<sup>1</sup>; Jonathan Rochon<sup>1</sup>; Mégane Moreau<sup>1</sup>; Serge Auger<sup>1</sup>; <sup>1</sup>Phytronix Technologies, Inc., Quebec, QC
- ThP 521 **Variable Temperature Electrospray Measurement of Enthalpy and Entropy of Tryptophan Binding to Ring Shaped Protein TRAP**; William J Moeller<sup>1,2</sup>; Mark P Foster<sup>3</sup>; Vicki H Wysocki<sup>2,3</sup>; <sup>1</sup>The Ohio State University, Columbus, OH; <sup>2</sup>Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH;

## THURSDAY POSTERS

- <sup>3</sup>Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH
- ThP 522 **Plasma-in-Droplet Ionization Mass Spectrometry**; Dmytro S Kulyk<sup>1</sup>; Purva S. Damale<sup>1</sup>; Abraham K. Badu-Tawiah<sup>1</sup>; <sup>1</sup>OSU, Columbus, OH
- ThP 523 **Triboelectric Nanogenerator-Coated Blade Spray Mass Spectrometry (TENG-CBS MS) for Volume-limited Drug Analysis**; Xin Ma<sup>1</sup>; Facundo M. Fernández<sup>1,2</sup>; <sup>1</sup>School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Petit Institute of Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA
- ThP 524 **Detection of ions generated in an intense pulsed EUV-light beam using different interfaces to a high-resolution TOF-MS**; Niklas Pengemann<sup>1</sup>; Sanna Benter<sup>1</sup>; Maja Hammelrath<sup>1</sup>; Joshua Rieger<sup>1</sup>; Franziska Schuler<sup>1</sup>; Adelind Elshani<sup>2</sup>; Ismael Gisch<sup>2</sup>; Linus Nagel<sup>2</sup>; Hendrik Kersten<sup>1</sup>; Sascha Brose<sup>2</sup>; Carlo Holly<sup>2</sup>; Peter Gust<sup>1</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany; <sup>2</sup>RWTH Aachen, Aachen, Germany
- ThP 525 **Lipophilic molecule analysis in a microtissue sample using supercritical fluid extraction/supercritical fluid chromatography-medium vacuum chemical ionization mass spectrometry**; Toshinobu Hondo<sup>1,2</sup>; Yumi Miyake<sup>1</sup>; Michisato Toyoda<sup>1</sup>; <sup>1</sup>Forefront Research Center, Graduate School of Science, Osaka University, Toyonaka, Japan; <sup>2</sup>MS-Cheminformatics, Inabe-Gun, Japan
- ThP 526 **Advancing Vacuum Matrix-Assisted Ionization (vMAI) Source for Multisample Introduction on a Portable Mass Spectrometer Using 3D Printing**; Chun-Yi Lin<sup>1</sup>; Milan Pophristic<sup>2</sup>; Charles McEwen<sup>3</sup>; Sarah Trimpin<sup>4</sup>; I-Chung Lu<sup>1</sup>; <sup>1</sup>Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan; <sup>2</sup>MSTM, LLC, Newark, DE; <sup>3</sup>University of the Sciences, Philadelphia, PA; <sup>4</sup>Wayne State University, Detroit, MI
- ThP 527 **An Autonomous, RGA Based Photoionization Mass Spectrometer for the Routine Detection of Atmospheric Trace Gases**; Kevin A. Wokosin<sup>1</sup>; Steven J. Kregel<sup>2</sup>; Robert L. McClain<sup>1</sup>; Timothy H. Bertram<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Bradley University, Peoria, IL
- ThP 528 **Probing ions from deeply embedded plasmas: From simulation to realization Investigation of a novel long distance ion transfer unit**; Sanna Benter<sup>1</sup>; Lena Mokros<sup>1</sup>; Markus Langner<sup>1</sup>; Niklas Pengemann<sup>1</sup>; Kersten Hendrik<sup>1</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>University of Wuppertal, Faculty of Mathematics and Natural Sciences, Wuppertal, Germany
- ThP 529 **Enhancing data quality in imaging and single-cell analysis through dopant-enriched nitrogen nebulizer gas**; Gábor Tóth<sup>1</sup>; Felix Friedrich<sup>1</sup>; Ingela Lanekoff<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden
- ThP 530 **Exploring a Stylus Pen as a Ion Source and Sampling Probe in Ambient Ionization Mass Spectrometry**; Yi-Ying Wu<sup>1</sup>; Yu-Chie Chen<sup>1</sup>; <sup>1</sup>National Yang Ming Chiao Tung University, Hsinchu City, Taiwan
- ThP 531 **A novel multifunctional ionization source for high-efficiency native mass spectrometry**; Anthony DeBastiani<sup>1</sup>; Stephen Valentine<sup>2</sup>; Amanda DeVor<sup>3</sup>; Peng Li<sup>3</sup>; Daud Sharif<sup>3</sup>; Sultan Mahmud<sup>3</sup>; Mohammed Rahman<sup>3</sup>; Chong Li<sup>3</sup>; Kushani Attanayake<sup>3</sup>; <sup>1</sup>WVU Department of Chemistry, Morgantown, WV; <sup>2</sup>Inviabragen, Inc., Morgantown, WV; <sup>3</sup>C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV
- ThP 532 **Simplified Drug Analysis: Optimizing Whole Blood Cartridge for Paper Spray Mass Spectrometry**; Greta Ren<sup>1</sup>; Nicholas E Manicke<sup>1</sup>; <sup>1</sup>IUPUI, Indianapolis, IN
- ThP 533 **Separation of steroid isomers via accelerated microdroplet derivatization enabled on a custom MALDESI source**; Paul Zerebinski<sup>1</sup>; Xizheng Diao<sup>2</sup>; Ruwan T Kurulugama<sup>3</sup>; Sarah M Stow<sup>3</sup>; Richard A Yost<sup>1</sup>; Timothy J. Garrett<sup>1,4</sup>; Boone M. Prentice<sup>1</sup>; <sup>1</sup>University of Florida Department of Chemistry, Gainesville, FL; <sup>2</sup>University of Florida, Department of Chemistry, Gainesville, FL; <sup>3</sup>Agilent Technologies, Santa Clara, CA; <sup>4</sup>University of Florida, Department of Pathology, Immunology, and Laboratory Medicine, Gainesville, Florida
- ThP 534 **Laser Ablation Electrospray of Proteins with Ion Mobility Mass Spectrometry**; Kelcey B. Hines<sup>1</sup>; Neda Feizi<sup>2</sup>; Touradj Solouki<sup>2</sup>; Kermit K. Murray<sup>1</sup>; <sup>1</sup>Louisiana State University, Baton Rouge, LA; <sup>2</sup>Baylor University, Waco, TX
- ThP 535 **Simulation of the pressure dependent Dynamic Ion Acceptance Volume (DIAV) of an electrically biased external ion sampling stage**; Markus Hübner<sup>1</sup>; Laura Lehmann<sup>1</sup>; Sanna Benter<sup>1</sup>; Hendrik Kersten<sup>1</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>Bergische Universität Wuppertal, Wuppertal, Germany
- ThP 536 **Kinetics of microsecond pulsed electrospray ionization**; Gavin Valdez<sup>1</sup>; Landon Vyhmeister<sup>1</sup>; Eric Davis<sup>1</sup>; <sup>1</sup>Whitworth University, Spokane, WA
- ThP 537 **Electric Field-Modulated Electrospray Ionization Mass Spectrometry for Quantity Calibration and Mass Tracking**; Pin-Chieh Hsu<sup>1</sup>; Pawel L. Urban<sup>2</sup>; <sup>1</sup>National Tsing Hua University, Hsinchu, Taiwan; <sup>2</sup>National Tsing Hua University, Hsinchu City, Taiwan
- ThP 538 **Fast, sensitive, robust, easy and quantitative direct ionization using air-permeable paper and vacuum matrix-assisted ionization (vMAI) mass spectrometry**; Hope Coffinberger<sup>1,2</sup>; Charles N. McEwen<sup>1,2</sup>; Sarah Trimpin<sup>1,3</sup>; <sup>1</sup>MSTM, LLC, Newark, DE; <sup>2</sup>Saint Joseph's University, Philadelphia, PA; <sup>3</sup>Wayne State University, Detroit, MI

### ION MOBILITY: FUNDAMENTALS 539-544

- ThP 539 **Ion chemistry simulation in Traveling Wave IMS using an open simulation framework (IDSIMF)**; Maja Hammelrath<sup>1</sup>; Michelle Rajkovic<sup>1</sup>; Walter Wißdorf<sup>1</sup>; Thorsten Benter<sup>1</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany
- ThP 540 **Tailoring Separations in SLIM with Traveling Wave Gradients**; Leonard Rorrer<sup>1</sup>; Jim Srock<sup>1</sup>; Ruwan T Kurulugama<sup>2</sup>; Miriam Fico<sup>1</sup>; Daniel DeBord<sup>1</sup>; <sup>1</sup>MOBILion Systems, Chadds Ford, PA; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- ThP 541 **Effect of charge sites on biomolecule separation in ion cloud profiling method**; Zhuofan Wang<sup>1</sup>; Shuai Li<sup>1</sup>; Liwen Liang<sup>1</sup>; Jiexun Bu<sup>2</sup>; Xinwei Liu<sup>2</sup>; Zheng Ouyang<sup>1</sup>; Xiaoyu Zhou<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China; <sup>2</sup>PURSPEC Technology (Beijing) Ltd., Beijing, China
- ThP 542 **Revisiting Protein Gas-Phase Unfolding: Contribution of the Mobile Proton Model through Covalent Chemical Modifications of Side Chains and Ion Mobility**; Thomas Tilmant<sup>1</sup>; Johann Far<sup>1</sup>; Edwin De Pauw<sup>1</sup>; Loïc Quinton<sup>1</sup>; <sup>1</sup>ULiège, Liège, Belgium
- ThP 543 **Ion Mobility Calculations of Flexible All-Atom Systems at Arbitrary Fields Using Two-Temperature Theory**; Farah Mubas-Sirah<sup>1</sup>; Viraj D. Gandhi<sup>1,2</sup>; Mohsen Latif<sup>1</sup>; Leyan Hua<sup>1</sup>; Amirreza Tootchi<sup>1</sup>; Carlos Larriba-Andaluz<sup>1</sup>; <sup>1</sup>Indiana University Purdue University Indianapolis, Indianapolis, IN; <sup>2</sup>Purdue University, West Lafayette, IN
- ThP 544 **Ion-gas collisional energy transfer between internal degrees of freedom at arbitrary fields and their effect on ion mobility**; Carlos Larriba Andaluz<sup>1</sup>; Viraj D Gandhi<sup>2,3</sup>; <sup>1</sup>IUPUI, Indianapolis, IN; <sup>2</sup>Indiana University Purdue University Indianapolis, Indianapolis, IN; <sup>3</sup>Purdue University, West Lafayette, IN

### ION MOBILITY: STRUCTURE

- 545-565ThP 545 **High-resolution Ion Mobility Mass Spectrometry (HRIM MS) Empowers Diastereomer Resolution in Synthetic Phosphorothioated Oligonucleotides**; Nnenna E. Dieke<sup>1</sup>; Joshua Shipman<sup>1</sup>; Cynthia Sommers<sup>1</sup>; Jason Rodriguez<sup>1</sup>; Deyi Zhang<sup>2</sup>; Darby Kozak<sup>2</sup>; Kui Yang<sup>1</sup>; <sup>1</sup>U.S. Food and Drug Administration, Saint Louis, MO; <sup>2</sup>U.S. Food and Drug Administration, Silver Spring, MD
- ThP 546 **Investigating Conformational Heterogeneity of Various Caspase-9 Maturation States**; Trisha W. Brady<sup>1</sup>; Vanessa L. Stahl<sup>1</sup>; Kristalle G. Cruz<sup>1</sup>; Jeanne A. Hardy<sup>1</sup>; Richard W Vachet<sup>1</sup>; <sup>1</sup>University of Massachusetts Amherst, Amherst, MA

## THURSDAY POSTERS

- ThP 547 **Understanding the Coordinative Selectivity of Glyphosate and AMPA Toward Divalent Metals by IM-MS and IM-IRMPD-MS;** Olivia Rusli<sup>1</sup>; Oscar H. Lloyd Williams<sup>1</sup>; Kevin Hes<sup>2</sup>; Sjors Bakels<sup>2</sup>; Anouk M. Rijs<sup>2</sup>; Nicole J. Rijs<sup>1</sup>; <sup>1</sup>UNSW Sydney, Kensington, Australia; <sup>2</sup>Division of BioAnalytical Chemistry, Vrije Universiteit Amsterdam, Amsterdam, Netherlands
- ThP 548 **Characterizing the Dipole Properties of Aligned Macromolecules by Next-Generation Low-Field Differential Ion Mobility Spectrometry Using Rectangular Waveforms with Orbitrap MS;** Hayden A Thurman<sup>1</sup>; Gordon A Anderson<sup>2</sup>; Alexandre A Shvartsburg<sup>1</sup>; <sup>1</sup>Wichita State University, Wichita, KS; <sup>2</sup>GAA Custom Electronics LLC, Kennewick, WA
- ThP 549 **Unveiling Novel L-to-D Amino Acid Residue Isomerization in Neuropeptides via Multi-faceted Single-Cell Mass Spectrometry;** GAOYUAN LU<sup>1</sup>; Vu Ngoc Huong Tran<sup>1</sup>; Wenxin Wu<sup>1</sup>; Zhijun Zhu<sup>1</sup>; Shuling Xu<sup>1</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI
- ThP 550 **Unraveling RNA Unfolding: A Comparative Study of RNA Collision Induced Unfolding and Solution-Phase Unfolding;** Anna G Anders<sup>1</sup>; Courteney R Dufrene<sup>1</sup>; Ingrid R Kilde<sup>2</sup>; Elizabeth E Tidwell<sup>3</sup>; Markos Koutmos<sup>2,4</sup>; Brandon T Ruotolo<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Michigan, Ann Arbor, Michigan; <sup>2</sup>Program in Chemical Biology, University of Michigan, Ann Arbor, Michigan; <sup>3</sup>Program in Biophysics, University of Michigan, Ann Arbor, Michigan; <sup>4</sup>Program in Biophysics, University of Michigan, Ann Arbor, Afghanistan
- ThP 551 **Metal Selectivity in High-Order Complexes of Depsipeptides Investigated by a Multimodal Approach;** Thanh D Do<sup>1</sup>; Emmanuel Nkyaagye<sup>2</sup>; Miranda N. Limbach<sup>2</sup>; <sup>1</sup>University of Tennessee, Knoxville, Knoxville, TN; <sup>2</sup>University of Tennessee Knoxville Chemistry Dept., Knoxville, TN
- ThP 552 **Atomic structure of an amyloidogenic segment of SOD1 with familial mutation linked to the progression of ALS;** Sarah S. Hirschbeck<sup>1</sup>; Michael R. Sawaya<sup>2</sup>; Joshua H. Jang<sup>3</sup>; Kristi L. Lazar Cantrell<sup>3</sup>; Thanh D. Do<sup>1</sup>; <sup>1</sup>University of Tennessee, Knoxville, TN; <sup>2</sup>University of California, Los Angeles, Los Angeles, CA; <sup>3</sup>Westmont College, Santa Barbara, CA
- ThP 553 **Flow Injection-Ion Mobility-Mass Spectrometry Tracks Structural Changes in Bacterial Microcompartment Components and Reveals Mechanisms of Oligomeric Structure Assembly;** Kiani Jeacock<sup>1</sup>; Claudia Mak<sup>2</sup>; Michael R. Armbruster<sup>1</sup>; Anthony Vecchiarelli<sup>2</sup>; Brandon T. Ruotolo<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Michigan, Ann Arbor, Michigan; <sup>2</sup>Department of Molecular, Cellular, and Developmental Biology, University of Michigan, Ann Arbor, Michigan
- ThP 554 **Structural Analysis of Protein Conformational Isomers via Ion Mobility and Collision Induced Unfolding;** Michael L Moore<sup>1</sup>; Richard W Vachet<sup>1</sup>; <sup>1</sup>University of Massachusetts Amherst, Amherst, MA
- ThP 555 **Identifying the Absolute Stereochemical Configuration of Biopolymer Building Blocks with Ion Mobility-Mass Spectrometry;** Mya M Brown<sup>1</sup>; Ron Orlando<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA
- ThP 556 **Structural elucidation and capture of the early steps in  $\alpha$ -synuclein aggregation revealed by ion mobility mass spectrometry;** Agathe Depraz Depland<sup>1,2</sup>; Raya Sadighi<sup>1,2</sup>; Anouk M. Rijs<sup>1</sup>; <sup>1</sup>Vrije Universiteit Amsterdam, Division of BioAnalytical Chemistry, Amsterdam, Netherlands; <sup>2</sup>Centre for Analytical Sciences Amsterdam, Amsterdam, Netherlands
- ThP 557 **Peptide conformational analysis by ion mobility mass spectrometry aids drug development;** Justin Mak<sup>1</sup>; Pierce Jessen<sup>1</sup>; Amin Famili<sup>1</sup>; Chris M Crittenden<sup>1</sup>; <sup>1</sup>Genentech, South San Francisco, CA
- ThP 558 **Detection of perfluoroalkyl carboxylic acid (PFCA) dimers in ion mobility spectrometry: using CCS-m/z trendlines to suggest their gas-phase conformation;** Aurore Schneiders<sup>1</sup>; Johann Far<sup>1</sup>; Lidia Belova<sup>2</sup>; Edwin De Pauw<sup>1</sup>; Adrian Covaci<sup>2</sup>; Gauthier Eppe<sup>1</sup>; <sup>1</sup>Liege University, Liège, Belgium; <sup>2</sup>University of Antwerp, Antwerp, Belgium
- ThP 559 **Average Charge State Analysis and Fourier Transform-Ion Mobility Provide Insights into the Conformational Dynamics of the GroEL-ATP Complex;** Kacie Evans<sup>1</sup>; He (Mirabel) Sun<sup>1</sup>; Robert L. Schrader<sup>1</sup>; Carter Lantz<sup>2</sup>; David H Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX
- ThP 560 **Ion mobility-based separations and selection for intact proteins enabled using native electrospray - Structures for Lossless Ion Manipulations (SLIM);** Jung Yun Lee<sup>1</sup>; Yehia M. Ibrahim<sup>1</sup>; Stephanie M. Thibert<sup>1</sup>; Christopher P. Harrilal<sup>1</sup>; Sandilya VB Garimella<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA
- ThP 561 **A modified SLIM-IM-QTOF for high resolution collision induced unfolding and native protein analysis;** Ruwan T. Kurulugama<sup>1</sup>; Sarah M. Stow<sup>1</sup>; Greg Kilby<sup>2</sup>; Daniel DeBord<sup>2</sup>; Harsha Gunawardena<sup>3</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>MOBILion Systems, Inc., Chadds Ford, PA; <sup>3</sup>JOHNSON AND JOHNSON, Spring House, PA
- ThP 562 **Accurate characterization of protein structures in the gas-phase: Combining ion-mobility, molecular dynamics simulations, and enhanced energy landscape sampling methods;** Viraj D Gandhi<sup>1,2</sup>; Morgan Lawrenz<sup>3</sup>; Iain D.G. Campuzano<sup>4</sup>; Carlos Larriba-Andaluz<sup>1</sup>; <sup>1</sup>Indiana University Purdue University Indianapolis, Indianapolis, IN; <sup>2</sup>Purdue University, West Lafayette, IN; <sup>3</sup>Schrödinger, Inc, San Diego, CA; <sup>4</sup>Amgen, Thousand Oaks, CA
- ThP 563 **Structural Identification of Small Molecules, Peptides, Proteins, and Complexes via nESI-TIMS-q-UVPD-FTICR MS/MS;** Samuel A Miller<sup>1</sup>; Kevin Jeanne Dit Fouque<sup>1</sup>; Miguel Santos<sup>1</sup>; Mark E Ridgeway<sup>2</sup>; Steve Van Orden<sup>3</sup>; Francisco A Fernandez-Lima<sup>1</sup>; <sup>1</sup>Florida International University, Miami, FL; <sup>2</sup>Bruker Scientific, LLC, Billerica, MA; <sup>3</sup>Bruker Daltonics Inc., Billerica, MA
- ThP 564 **Ion mobility reveals intriguing solvent effects on lossless intramolecular proton transfers in gaseous ion ensembles;** Athula B. Attygalle<sup>1</sup>; Meenu Kumar<sup>1</sup>; <sup>1</sup>Stevens Institute of Technology, Hoboken, NJ
- ThP 565 **All Multispecific-Antibodies Undergo Large and Measurable Levels of Gas-Phase Collapse;** Iain D G Campuzano<sup>1</sup>; CHEN-CHUN CHEN<sup>2</sup>; <sup>1</sup>Amgen Inc., Thousand Oaks, CA; <sup>2</sup>Eli Lilly and Company, Indianapolis, IN

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- ThP 566 **Optimization of LC-MS Method Development for Efficient Quantification of CYP Metabolites: A QTOF based Mass Spectrometry Approach;** Zarna A Raichura<sup>1</sup>; Kabre Heck<sup>1</sup>; Angela Calderon<sup>1</sup>; <sup>1</sup>Auburn University, Auburn, AL
- ThP 567 **Influence of gas impurities on electrospray spectra background noise;** Tomasz Bienkowski<sup>1,2</sup>; Konrad Kowalski<sup>2,3</sup>; <sup>1</sup>LNI SWISSGAS EE sp. z o.o., Warszawa, Poland; <sup>2</sup>Masdiag Sp. z o.o., Warsaw, Poland; <sup>3</sup>MS Ekspert Sp. z o.o., Gdańsk, Poland
- ThP 568 **Method development and analytical validation for key phospholipids in pharmaceutical raw materials for total parenteral nutrition products using UPLC-Orbitrap MS;** Mark Dennis C Retrato<sup>1</sup>; Kumari Ubhayasekera<sup>1</sup>; Jonas Bergquist<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden
- ThP 569 **Enhanced Online Post-Column Reactions Driven by Supersonic Microdroplet Electrospray for Characterizing Disulfide Linkages and Quantifying DNA Adducts Using Microflow-LC-MS2;** Shu-Hui Chen<sup>1</sup>; Husam Kafeenah<sup>1</sup>; Quynh-Trang Do<sup>1</sup>; Fung-Yu Chen<sup>1</sup>; <sup>1</sup>National Cheng Kung University, Tainan, Taiwan
- ThP 570 **Method Development of Sample Preparation and HPLC Separation for the Characterization of Peptide-RNA Conjugates via LC-MS;** Christopher Kovach<sup>1</sup>; Guihong Qi<sup>1</sup>; Xianyin Lai<sup>1</sup>; <sup>1</sup>Eli Lilly & Company, Indianapolis, IN
- ThP 571 **Quality Control of Newly Synthesized Small Molecules and Peptides Using High Throughput UPLC-MS;** Wilfredo Pinto<sup>1</sup>; Foster Tenkorang<sup>1</sup>; <sup>1</sup>Merck, Rahway, NJ

## THURSDAY POSTERS

- ThP 572 **Agilent RoHS Compliant Ion Injector for LCMS Single Quadrupole and Triple Quadrupole Instruments**; Samuel Haddad<sup>1</sup>; Jennifer Sanderson<sup>2</sup>; Paul Tripp<sup>3</sup>; <sup>1</sup>Agilent Technologies, Wilmington, DE; <sup>2</sup>Agilent Technologies Inc., Santa Clara, CA; <sup>3</sup>Agilent Technologies, Santa Clara, CA
- ThP 573 **Dipolarity Polarity Component of the Mobile Phase: A Crucial Factor in the Separation of Bile Acid Enantiomers in RPLC-MS**; Mst Ummul Khair<sup>1</sup>; David Anderson<sup>2</sup>; <sup>1</sup>Cleveland State University, Cleveland, OH; <sup>2</sup>Cleveland State University, CLEVELAND, OH
- ThP 574 **Lipid Characterization of Extracellular Vesicles Released by Drug-resistant Leishmania Parasites**; Erica Kim<sup>1</sup>; Ana Victoria Ibarra-Meneses<sup>2</sup>; Alisa Hui<sup>1</sup>; Christopher Fernandez Prada<sup>2</sup>; Tao Huan<sup>1</sup>; <sup>1</sup>University of British Columbia, Vancouver, BC; <sup>2</sup>University of Montreal, Montreal, QC
- ThP 575 **Troubleshooting and Counteracting Quetiapine-Induced Interference in LC-MS/MS analysis**; Jongsun Joo<sup>1</sup>; Ju Hyeong Lee<sup>1</sup>; Jikyo Lee<sup>1</sup>; Sang Hoon Song<sup>1</sup>; <sup>1</sup>Seoul National University Hospital, Seoul, South Korea
- ThP 576 **An Alternative Approach for NDMA Quantification in Metformin Final Product by LC/MS Single Quadrupole**; Lucas Lima Zanin<sup>1</sup>; Marcos Albieri Pudenzi<sup>1</sup>; Ichiro Hirano<sup>2</sup>; <sup>1</sup>Shimadzu do Brasil, Barueri, Brazil; <sup>2</sup>Shimadzu do Brasil, Barueri, Brazil
- ThP 577 **Enabling faster MRM while maintaining instrument robustness**; David Cox<sup>1</sup>; Yang Kang<sup>1</sup>; Ian Moore<sup>1</sup>; Holly Lee<sup>1</sup>; Michael Deng<sup>1</sup>; <sup>1</sup>SCIEX, Concord, ON
- ThP 578 **Pushing the flexibility of Multi-task analysis: The challenges of an MS facility are wide-ranging projects on limited instrumentation**; Reynard A Spiess<sup>1</sup>; Katherine Hollywood<sup>1</sup>; Aliaksandr Baidak<sup>1</sup>; Jaleel Miyan<sup>1</sup>; Harmesh Aojula<sup>1</sup>; Shaymaa Mudhaffer<sup>1</sup>; Elen Clayton<sup>1</sup>; Vishal Kawale<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, United Kingdom
- ThP 579 **A 3D-printed serpentine column for size exclusion chromatography separations with mass spectrometric detection**; Olanrewaju Awowemi<sup>1</sup>; Jing Wang<sup>1</sup>; Madison Pursell<sup>1</sup>; Amanda DeVor<sup>1</sup>; Riley White<sup>1</sup>; Stephen J Valentine<sup>1</sup>; Peng Li<sup>1</sup>; <sup>1</sup>West Virginia University, Morgantown, WV
- ThP 580 **Development of a Desalination Tube for an On-line LC/MS Analysis**; Yutaka Takahashi<sup>1,2,3</sup>; Sachiki Shimizu<sup>3</sup>; Takumi Sakamoto<sup>1</sup>; Mitsutoshi Setou<sup>1</sup>; <sup>2</sup>Hamamatsu University School of Medicine, Shizuoka, Japan; <sup>3</sup>Preppers Co. Ltd, Shizuoka, Japan; <sup>3</sup>MS-Solutions Co. Ltd., Tokyo, Japan
- ThP 581 **High-Throughput Quantification of Vitamin D Metabolites in Dried Blood Spots**; Keeley Jo Alexander<sup>1</sup>; Kavinda DeSilva<sup>1</sup>; Frances Morris<sup>1</sup>; Zane Hauck PhD<sup>1</sup>; <sup>1</sup>Molecular Testing Labs, Vancouver, WA
- ThP 582 **Lifetime Testing of Novel RoHS Compliant Ion Injectors with Real-time Early Maintenance Feedback (EMF) Diagnostic Monitoring on Multiple LC/TQ Platforms**; Sampada Borkar<sup>1</sup>; Michael B Pastor<sup>1</sup>; Ryan Rademacher<sup>1</sup>; Paul Tripp<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA
- ThP 583 **Antisense oligonucleotide extraction optimization reveals significant differences between non-human primate spinal cord, mouse spinal cord, and mouse brain tissue homogenates**; Brandon M Davies<sup>1</sup>; Brandon Wilcock<sup>1</sup>; Terry Fang<sup>2</sup>; Brian Bettencourt<sup>2</sup>; Troy Voelker<sup>1</sup>; <sup>1</sup>Aliri Bioanalysis, Salt Lake City, UT; <sup>2</sup>Third Rock NewCo, Boston, USA, MA
- ThP 584 **New HESI sprayer design for improved precision and robustness across all source temperature/gas ranges**; Charles Maxey<sup>1</sup>; Cornelia Boeser<sup>1</sup>; Neloni Wijeratne<sup>1</sup>; Eloy R. Wouters<sup>1</sup>; Brian Adamson<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 585 **Evaluating Diverse Modalities for LC-MS/MS Quantitation Across Three Sciex Triple Quadrupole Platforms**; Carla Camou-Sainz<sup>1</sup>; Darian Bartkowski<sup>1</sup>; Alyssa Gillies<sup>1</sup>; <sup>1</sup>Takeda, San Diego, CA
- ThP 586 **Open-tubular trap columns: towards simple and robust liquid chromatography separations for single-cell proteomics**; Siji Huang<sup>1</sup>; Kei Webber<sup>1</sup>; Thy Truong<sup>1</sup>; Jacob Heninger<sup>1</sup>; Ryan T. Kelly<sup>1,2</sup>; <sup>1</sup>Brigham Young University, Provo, UT; <sup>2</sup>MicrOmics Technologies, Spanish Fork, UT
- ThP 587 **Trace level estimation of N-Nitroso Isavuconazonium Sulphate in Isavuconazonium Sulphate API using liquid chromatography and nominal mass tandem mass spectrometry**; Ian Edwards<sup>1</sup>; Saikat Bhattacharya<sup>2</sup>; Prasanth Joseph<sup>2</sup>; Vivek Dhyani<sup>3</sup>; Saikat Banerjee<sup>4</sup>; <sup>1</sup>Agilent Technologies Inc., Santa Clara, CA; <sup>2</sup>Agilent technologies, Bangalore, India; <sup>3</sup>Agilent Technologies, Mumbai, India; <sup>4</sup>Agilent Technologies, Hyderabad, India
- ThP 588 **Sensitive and selective quantitation of N-nitroso dabigatran etexilate impurity (NDSRI) in dabigatran drug substance at picogram levels using LC/MS/MS**; Parul Angrish<sup>1</sup>; Preeti Bharatiya<sup>2</sup>; Prasanth Joseph<sup>2</sup>; Vivek Dhyani<sup>3</sup>; Saikat Banerjee<sup>4</sup>; Kannan Balakrishnan<sup>2</sup>; <sup>1</sup>Agilent Technologies Inc., Santa Clara, USA; <sup>2</sup>Agilent Technologies Inc., Bangalore, India; <sup>3</sup>Agilent Technologies Inc., Mumbai, India; <sup>4</sup>Agilent Technologies Inc., Hyderabad, India
- ThP 589 **Utilization of the speed, sensitivity and accuracy of the ZenoTOF 7600 to enhance protein identifications from packed emitter columns**; Sri Ramarathinam<sup>1</sup>; Aaron Poth<sup>2</sup>; Mohammadreza Dorvash<sup>1</sup>; Patricia Illing<sup>1</sup>; Jarrod Sandow<sup>2</sup>; Anthony Purcell<sup>1</sup>; <sup>1</sup>Monash University, Clayton, Australia; <sup>2</sup>IonOpticks, Fitzroy, Australia
- ThP 590 **Determination of Paraquat in Drinking Water by LCMS-2050**; Marilia Santoro Cardoso<sup>1</sup>; Marcos A Pudenzi<sup>2</sup>; Luisa B Ambrosio<sup>2</sup>; Ichiro Hirano<sup>2</sup>; <sup>1</sup>Shimadzu do Brasil, Barueri - SP, Brazil; <sup>2</sup>Shimadzu do Brasil, Barueri, Brazil
- ThP 591 **Simultaneous quantitation of N-nitrosamines and NDSRIs in formulation samples by using a DUIS ionization source in LC-MS/MS**; Nitish Ramchandra Suryawanshi<sup>1</sup>; Samruddha Chavan<sup>1</sup>; Nitin Shukla<sup>1</sup>; Devika Tupe<sup>1</sup>; Siddhesh Ghadi<sup>1</sup>; Shalu Nair<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; Pratap Rasam<sup>1</sup>; <sup>1</sup>Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- ThP 592 **Quantification of potentially toxic chemicals in simulated leachate from four widely used tire-derived materials by LC/MS/MS**; Jonathan Navarro Ramos<sup>1</sup>; John D. Atkinson<sup>2</sup>; Joshua Wallace<sup>1</sup>; Diana S Aga<sup>1</sup>; James Lang<sup>2</sup>; Phillip Zimako Onyeme<sup>2</sup>; <sup>1</sup>Department of Chemistry, The State University of New York at Buffalo, Buffalo, NY; <sup>2</sup>Department of Civil, Structural, and Environmental Engineering, The State University of New York at Buffalo, Buffalo, NY
- ThP 593 **Stability indicating LC-MS/MS method for estimation of Bromocriptine mesylate in human plasma application to a bioequivalence study**; Narendra Kumar Reddy Kolli<sup>1</sup>; Swetha Polagani<sup>1</sup>; Arya Lakshmi Mariseti<sup>2</sup>; <sup>1</sup>Sri Vani School Of Pharmacy, Vijayawada, India; <sup>2</sup>Delhi Pharmaceutical Sciences and Research University, New Delhi, India
- ThP 594 **Estimation of Levetiracetam in Human K2EDTA Plasma in range from 0.253 µg/mL to 35.060 µg/mL by using LC-MS/MS**; Swetha Polagani<sup>1</sup>; Narendra Kumar Reddy Kolli<sup>2</sup>; Murali Krishna Kumar Muthyala<sup>3</sup>; <sup>1</sup>Sri Vani School Of Pharmacy, Vijayawada., India; <sup>2</sup>Sri Vani School Of Pharmacy, Vijayawada, India; <sup>3</sup>Andhra University College Of Pharmaceutical Sciences, Visakhapatnam, India

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- ThP 595 **The Innovation Solution of Eicosanoids and Related Oxylipins Profiles as Biomarkers by LC-MS/MS in Uterine Fibroids Disease**; Ting-Li Han<sup>1</sup>; Xin Wang<sup>1</sup>; Xiao-Rong Ran<sup>2</sup>; Yue Song<sup>3</sup>; Shan-An Chan<sup>4</sup>; <sup>1</sup>State Key Laboratory of Ultrasound in Medicine and Engineering, College of Biomedical Engineering, Chongqing Medical University, Chongqing, China; <sup>2</sup>Agilent Technologies Inc., Beijing, China; <sup>3</sup>Agilent Technologies Inc., Shanghai, China; <sup>4</sup>Agilent Technologies Inc., Taipei, China



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- ThP 596 **Estimation of positional lipid isomers in a biological mixture using Parallel Reaction Monitoring (prm) and isomer quantification model;** Dhanwin Baker<sup>1</sup>; Laura Bindila<sup>1</sup>; <sup>1</sup>University Medical Center of Mainz, Mainz, Germany
- ThP 597 **Application of Targeted Lipidomics to Determine Changes in the Plasma Lipidome of Male Rats Follow Repeat Oral Administration of Methapyrilene;** Robert Plumb<sup>1</sup>; Ian D Wilson<sup>2</sup>; Andrew Leightner<sup>3</sup>; Anthony J Midey<sup>3</sup>; Steven K Lai<sup>3</sup>; Roy Martin<sup>4</sup>; <sup>1</sup>Waters, Milford, MA; <sup>2</sup>Imperial College London, London, United Kingdom; <sup>3</sup>Waters Corporation, Milford, MA; <sup>4</sup>Waters Corporation, Milford, Massachusetts
- ThP 598 **Intramolecular Paternò-Büchi reaction coupled with isobaric tagging for parallel quantitation of fatty acids at multiple structural levels;** Lipeng Qiao<sup>1</sup>; Hengxue Shi<sup>1</sup>; Yichun Wang<sup>1</sup>; Yu Xia<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing, China
- ThP 599 **LICAR2: automated isotopic correction tool for targeted lipidomic data acquired with class-based chromatographic separations using multiple reaction monitoring;** Liang Gao<sup>1</sup>; Shanshan Ji<sup>1</sup>; Amaury Cazenave-Gassiot<sup>1</sup>; Bo Burla<sup>1</sup>; <sup>1</sup>National University of Singapore, Singapore, Singapore
- ThP 600 **Targeted lipidomics of a randomized crossover trial with human subjects;** Nara Marella<sup>1</sup>; Matthäus Metz<sup>2</sup>; Marianna Beghini<sup>2</sup>; Peter Wolf<sup>2</sup>; Lorenz Pflieger<sup>2</sup>; Martina Hackl<sup>2</sup>; Magdalena Bastian<sup>2</sup>; Angelika Freudenthaler<sup>2</sup>; Juergen Harreiter<sup>2</sup>; Maximilian Zeyda<sup>3</sup>; Sabina Baumgartner-Parzer<sup>2</sup>; Rodrig Marculescu<sup>4</sup>; Thomas Hannich<sup>5</sup>; Georg Gyoerig<sup>6</sup>; Gabriela Berlakovich<sup>6</sup>; Michael Roden<sup>7</sup>; Micahel Krebs<sup>2</sup>; Robert Risti<sup>8</sup>; Aivar Lökene<sup>9</sup>; Michael Trauner<sup>10</sup>; Alexandra Kautzky-Willer<sup>2</sup>; Martin Krššák<sup>2</sup>; Herbert Stangl<sup>11</sup>; Clemens Fürsinn<sup>2</sup>; Thomas Scherer<sup>2</sup>; <sup>1</sup>CeMM Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria; <sup>2</sup>Division of Endocrinology and Metabolism, Department of Internal Medicine III, Medical University of Vienna, Vienna, Austria; <sup>3</sup>Clinical Division of Pediatric Pulmonology, Allergology and Endocrinology, Department for Pediatrics and Adolescent Medicine, Comprehensive Center for Pediatrics, Medical University of Vienna, Vienna 1090, Austria, Vienna, Austria; <sup>4</sup>Department of Laboratory Medicine, Medical University of Vienna, Vienna 1090, Austria, Vienna, Austria; <sup>5</sup>CeMM Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria; <sup>6</sup>Division of Transplantation, Department of Surgery, Medical University of Vienna, Vienna 1090, Austria, Vienna, Austria; <sup>7</sup>Division of Endocrinology and Diabetology, Medical Faculty and University Hospital, Heinrich Heine University, Düsseldorf 40225, Germany, Duesseldorf, Germany; <sup>8</sup>Department of Chemistry, Tallinn University of Technology, Tallinn 12618, Estonia, Estonia, Estonia; <sup>9</sup>Department of Chemistry, Tallinn University of Technology, Tallinn 12618, Estonia, Estonia, Austria; <sup>10</sup>Division of Gastroenterology and Hepatology, Department of Internal Medicine III, Medical University of Vienna, Vienna 1090, Austria, Vienna, Austria; <sup>11</sup>Institute of Medical Chemistry, Center for Pathobiochemistry and Genetics, Medical University of Vienna, Vienna 1090, Austria, Vienna, Austria
- ThP 601 **Investigation of PLA2 Inhibitors' Influence on Enzymatic and Non-Enzymatic Oxidized Phospholipids in Immortalized Microglial Cells;** Sazia Arefin Kachi<sup>1</sup>; Yulemni Morel<sup>1</sup>; Amir Mehrabani Tabari<sup>2</sup>; Nivedita Hegdekar<sup>2</sup>; Chinmoy Sarkar<sup>2</sup>; Marta M. Lipinski<sup>2</sup>; Jace W. Jones<sup>1</sup>; <sup>1</sup>University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD; <sup>2</sup>University of Maryland, School of Medicine, Department of Anesthesiology, Baltimore, MD
- ThP 602 **LC-ESI-MS/MS Analysis of Oxygenated PUFA-PE in ferroptotic naive PMN and PMN-MDSC from bone marrow and spleens of tumor-bearing mice;** Vladimir A Tyurin<sup>1</sup>; Yulia Y Tyurina<sup>1</sup>; Rina Kim<sup>2</sup>; Ayumi Hashimoto<sup>3</sup>; Valerian E Kagan<sup>4</sup>; Dmitry I Gabrilovich<sup>3</sup>; Yulia Nefedova<sup>2</sup>; <sup>1</sup>University of Pittsburgh, Pittsburgh, PA; <sup>2</sup>University of Pennsylvania, Philadelphia, PA; <sup>3</sup>AstraZeneca, Gaithersburg, MD; <sup>4</sup>University of Pittsburgh, Pittsburgh, Pennsylvania; <sup>5</sup>Wistar Institute, Philadelphia, PA
- ThP 603 **The lipoprotein-associated phospholipase A2 inhibitor Darapladib sensitises cancer cells to ferroptosis by remodelling lipid metabolism;** Seoyoung Jang<sup>1</sup>; Mihee Oh<sup>2</sup>; Ji-Yoon Lee<sup>2</sup>; Eun-Woo Lee<sup>2</sup>; Geum-Sook Hwang<sup>1</sup>; <sup>1</sup>Korea Basic Science Institute, Seoul, South Korea; <sup>2</sup>Korea Research Institute of Bioscience and Biotechnology, Daejeon, South Korea
- ThP 604 **Investigate Skin Fibroblasts Lipidome Changes in Optic Disc Drusen Using a Comprehensive Targeted LC-dMRM Method;** Mengying Fu<sup>1</sup>; Yujin Dai<sup>1</sup>; Karanvir Kaushal<sup>2</sup>; Yaping Joyce Liao<sup>2</sup>; <sup>1</sup>Sarafan ChEM-H, Stanford University, Stanford, CA; <sup>2</sup>Department of Ophthalmology, Stanford University, Stanford, CA
- ThP 605 **A high efficiency quantitation method for aldehyde-containing compounds based on chemical isotope-coded derivatization;** XIAOHUI FENG<sup>1</sup>; Zhenghua Rao<sup>1</sup>; Yaxiong Jia<sup>1</sup>; <sup>1</sup>Institute of Animal Sciences, CAAS, Beijing, China
- ThP 606 **Elevated levels of arachidonic acid containing lipids underlie cardiovascular disease risk in White and Black Females;** Raghav Jain<sup>1</sup>; Jessica W Davidson<sup>1</sup>; Dominique A Baldwin<sup>1</sup>; Judith Simcox<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Biochemistry, Madison, WI
- ThP 607 **Comprehensive shotgun lipidomics workflow using SLA platform and LipStR for the lipid profiling of human milk;** Weng Wong<sup>1</sup>; James Joubert<sup>1</sup>; Meena Choi<sup>1</sup>; William Dishen Liu<sup>1</sup>; Anatoly Belov<sup>1</sup>; Jay Leone<sup>1</sup>; Wendy Sandoval<sup>1</sup>; Qingling Li<sup>1</sup>; <sup>1</sup>Genentech, South San Francisco, CA
- ThP 608 **Unleashing High Sensitivity: NanoLC Monolithic Columns in 4D Metabolomics and Lipidomics;** Tina McGuire<sup>1</sup>; Michael Krawitzky<sup>2, 3</sup>; Erica Marie Forsberg<sup>1</sup>; Goran Mitulovic<sup>3</sup>; Matthew R Lewis<sup>4</sup>; <sup>1</sup>Bruker Scientific, LLC, Billerica, MA; <sup>2</sup>Bruker Daltonics, San Jose, CA; <sup>3</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>4</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany
- ThP 609 **Optimization of a sensitive method for quantifying dicarboxylic acids using liquid chromatography tandem mass spectrometry;** Joby Jose<sup>1</sup>; Alfred N Fonteh<sup>1</sup>; <sup>1</sup>Huntington Medical Research Institutes, Pasadena, CA
- ThP 610 **High-Throughput Mass Spectrometry Assay Platform for Characterizing Selectivity of Small Molecule Inhibitors Against Multiple Enzymes in the Cholesterol Biosynthesis Pathway;** Ronghai Cheng<sup>1</sup>; Reza Nemati Josheghani<sup>1</sup>; Daniel Tekverk<sup>1</sup>; Howard Jones<sup>1</sup>; Martin Himmelbauer<sup>1</sup>; <sup>1</sup>Biogen, Cambridge, MA
- ThP 611 **Profiling of glycosphingolipids and gangliosides from dried bloodspots for diagnosis of inherited genetic disorders;** Jinyong Kim<sup>1</sup>; Seul Kee Byeon<sup>1</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN
- ThP 612 **Pyridine deuteration for the synthesis of Isotope-Coded-Derivatization agent with a fixed charge and its application for fatty acids analysis;** Jorge Gabriel Ascencio Delgado<sup>1</sup>; Katarzyna Dorota Wrobel<sup>1</sup>; Oracio Serrano Torres<sup>1</sup>; Kazimierz Wrobel<sup>1</sup>; <sup>1</sup>University of Guanajuato, Guanajuato, Mexico
- ThP 613 **Base Hydrolysis (or Not) for Targeted Sphingolipid Quantitation;** Josie Daldegan Rezende<sup>1</sup>; Yuanyuan Ji<sup>1</sup>; Anh Tran<sup>1</sup>; Jace W. Jones<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore, Baltimore, MD
- ThP 614 **Identifying Dysregulated Lipids in Human Brain of Alzheimer's Disease and their Effects on Biological Pathways;** Akeem Sanni<sup>1</sup>; Andrew I Bennett<sup>1</sup>; Moyinoluwa Adeniyi<sup>1</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, Texas
- ThP 615 **Ferrolaxins inhibit phosphatidylethanolamine oxidation catalyzed by 15LOX/PEBP1 complex in vitro and in vivo and mitigate ferroptosis;** Yulia Y. Tyurina<sup>1</sup>; Haider H. Dar<sup>1</sup>; Karolina Mikulska-Ruminska<sup>2</sup>; Diane K. Luci<sup>3</sup>; Adam Yasgar<sup>3</sup>; Svetlana N. Samovich<sup>4</sup>; Kapralov A Alexander<sup>1</sup>;

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- Austin B. Souryavong<sup>1</sup>; Vladimir A. Tyurin<sup>1</sup>; Andrew A Amoscato<sup>1</sup>; Louis J. Sparvero<sup>1</sup>; Ecem Saritas<sup>1</sup>; Mert Akdogan<sup>1</sup>; Michael W Epperly<sup>1</sup>; Galina V. Shurin<sup>1</sup>; Melissa Standley<sup>5</sup>; Theodore R Holman<sup>5</sup>; Claudette M. St. Croix<sup>1</sup>; Simon C. Watkins<sup>1</sup>; Andrew P. VanDemark<sup>1</sup>; Sandeep Rana<sup>3</sup>; Alexey V. Zakharov<sup>3</sup>; Anton M. Simeonov<sup>3</sup>; Rama K. Mallampalli<sup>6</sup>; Sally E. Wenzel<sup>1</sup>; Joel S. Greenberger<sup>1</sup>; Ganesha Rai<sup>3</sup>; Hülya Bayir<sup>4</sup>; Ivet Bahar<sup>7</sup>; Valerian E Kagan<sup>1</sup>; <sup>1</sup>University of Pittsburgh, Pittsburgh, PA; <sup>2</sup>Nicolaus Copernicus University, Bydgoszcz, Poland; <sup>3</sup>National Center for Advancing Translational Sciences (NCATS), Rockville, MD; <sup>4</sup>Columbia University Irving Medical Center, New York, NY; <sup>5</sup>University of California Santa Cruz, Santa Cruz, CA; <sup>6</sup>The Ohio State University, Columbus, OH; <sup>7</sup>Stony Brook University, Stony Brook, NY
- ThP 616 **Impact of chronic exposure to environmentally relevant micro/nanoplastics on mouse lipidome by D2O metabolic labeling**; Jonghyun Kim<sup>1</sup>; Jinyoung Park<sup>1</sup>; Hyoun Hyoung Jang<sup>1</sup>; Sokkhorhn Phorn<sup>1</sup>; Tae-Young Kim<sup>1</sup>; <sup>1</sup>School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea
- ThP 617 **Targeted method of polyprenols and dolichols using ion trap-based higher energy collision-induced dissociation**; Seul Kee Byeon<sup>1</sup>; Jinyong Kim<sup>1</sup>; Rahul R Deshpande<sup>2</sup>; Susan S. Bird<sup>2</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN; <sup>2</sup>ThermoFisher Scientific, San Jose, CA
- ThP 618 **Breaking Limits: Nanoscale LC-TIMS-MS Empowers Low Sample Volume Single-Cell 4D-Lipidomics**; Rebekah J Woolsey<sup>1</sup>; Michael Krawitzky<sup>2, 3</sup>; Irina Maerki<sup>3</sup>; Florian Busch<sup>3</sup>; Sven W Meyer<sup>4</sup>; Erica Marie Forsberg<sup>5</sup>; Claudia Martinelli<sup>3</sup>; Jean-François Greisch<sup>3</sup>; Matthew R Lewis<sup>4</sup>; <sup>1</sup>University of Nevada Reno, Reno, NV; <sup>2</sup>Bruker Daltonics, San Jose, CA; <sup>3</sup>Bruker Switzerland AG, Faellanden, Switzerland; <sup>4</sup>Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; <sup>5</sup>Bruker Scientific, LLC, Billerica, MA
- ThP 619 **Fatty acids positional isomers quantification using nanospray Supercritical Fluid Chromatography-Mass Spectrometry (nSFC-MS)**; Mahmoud Elhousseiny Abdelrahman Mostafa<sup>1</sup>; John R Boughton<sup>2</sup>; James P Grinias<sup>2</sup>; James Edwards<sup>1</sup>; <sup>1</sup>Saint Louis University, Saint Louis, MO; <sup>2</sup>Rowan University, Glassboro, New Jersey
- ThP 620 **Comprehensive Analysis of Signaling Lipids in Biological Matrices Using Metal-free LC-MS/MS**; Stefanie Rubenzucker<sup>1,2</sup>; Mailin-Christin Manke<sup>3,4</sup>; Rainer Lehmann<sup>5</sup>; Alice Assinger<sup>6</sup>; Oliver Borst<sup>3,4</sup>; Robert Ahrends<sup>1</sup>; <sup>1</sup>Department of Analytical Chemistry, University of Vienna, Vienna, Austria; <sup>2</sup>Vienna Doctoral School in Chemistry (DoSChem), University of Vienna, Vienna, Austria; <sup>3</sup>Department of Cardiology and Angiology, University of Tuebingen, Tuebingen, Germany; <sup>4</sup>DFG Heisenberg Group Cardiovascular Thromboinflammation and Translational Thrombocardiology, University of Tuebingen, Tuebingen, Germany; <sup>5</sup>Institute for Clinical Chemistry and Pathobiochemistry, Department for Diagnostic Laboratory Medicine, University Hospital Tuebingen, Tuebingen, Germany; <sup>6</sup>Department of Vascular Biology and Thrombosis Research, Centre of Physiology and Pharmacology, Medical University of Vienna, Vienna, Austria
- ThP 621 **High-throughput, quantitative targeted lipidomic method for large-scale measurement of lipids in human plasma samples**; Yuanyuan Ji<sup>1</sup>; Yulemni Morel<sup>1</sup>; Anh Tran<sup>1</sup>; Jace W. Jones<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore, Baltimore, MD
- ThP 622 **Towards targeted and quantitative 4D Lipidomics - From PASEF to prm-PASEF**; Edward Rudt<sup>1</sup>; Viola Jeck<sup>2</sup>; Nikolas Kessler<sup>2</sup>; Christian Müller<sup>2</sup>; Ilmari Krebs<sup>2</sup>; Heiko Neuweger<sup>2</sup>; Heiko Hayen<sup>1</sup>; <sup>1</sup>University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; <sup>2</sup>Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- ThP 623 **The lysophosphatidylcholine is an essential and versatile source for de novo phospholipids' biosynthesis in Plasmodium falciparum**; Corinne BURE<sup>1</sup>; Quentin Chevalier<sup>2</sup>; Sharon Wein<sup>2</sup>; Rachel Cerdan<sup>2</sup>; <sup>1</sup>CNRS - IECB, Pessac, France; <sup>2</sup>Montpellier University, MONTPELLIER, France
- ThP 624 **Wide-scope targeted analysis of bioactive lipids by LC/MS/MS**; Kohta Nakatani<sup>1</sup>; Yoshihiro Izumi<sup>1</sup>; Hironobu Umakoshi<sup>2</sup>; Maki Yokomoto-Umakoshi<sup>2</sup>; Tomoko Nakaji<sup>1</sup>; Hiroki Kaneko<sup>2</sup>; Hiroshi Nakao<sup>2</sup>; Yoshihiro Ogawa<sup>2</sup>; Kazutaka Ikeda<sup>3</sup>; Takeshi Bamba<sup>1</sup>; <sup>1</sup>Medical Institute of Bioregulation, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka-shi, Japan; <sup>2</sup>Department of Medicine and Bioregulatory Science, Graduate School of Medical Sciences, Kyushu University, Fukuoka, Japan; <sup>3</sup>Kazusa DNA Research Institute, 2-6-7 Kazusakamatari, Kisarazu, Japan
- ThP 625 **The New Normal: Evidence for why we should stop using protein concentration for lipid normalization in quantitative lipidomics**; Kari B Basso<sup>1</sup>; Laura Bailey<sup>2</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>University of Florida, Department of Chemistry, Gainesville, FL
- ThP 626 **LC-MRM-MS profiling of oxylipins and fatty acids in human milk after hydrolysis**; Liping Yang<sup>1</sup>; Jaewoo Choi<sup>1</sup>; David C. Dallas<sup>2</sup>; Jan F. Stevens<sup>3,4</sup>; Claudia S. Maier<sup>1,4</sup>; <sup>1</sup>Department of Chemistry, Oregon State University, Corvallis, OR; <sup>2</sup>Nutrition Program, College of Health, Oregon State University, Corvallis, OR; <sup>3</sup>Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR; <sup>4</sup>Linus Pauling Institute, Oregon State University, Corvallis, OR
- ThP 627 **LC-MS/MS analysis of glucosylceramides (GlcCer) and glucosylsphingosine (GlcSph) in L444P fibroblast cells**; Nicole E Bebrin<sup>1</sup>; Sho Sato<sup>1</sup>; Shin-ichi Matsumoto<sup>2</sup>; Hiroshi Sugimoto<sup>1</sup>; <sup>1</sup>Takeda Pharmaceuticals, Cambridge, MA; <sup>2</sup>Takeda Pharmaceutical Company Limited, Fujisawa, Japan

### MALDI: APPLICATIONS 628-638

- ThP 628 **Determining the stability of botulism clinical specimens using MALDI-TOF mass spectrometry**; Victoria Foltz<sup>1</sup>; Kiara Gonzalez-Colon<sup>1,2</sup>; Janet Dykes<sup>1</sup>; Andre Hopkins<sup>1</sup>; Carolina Luquez<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA; <sup>2</sup>ASRT, Inc, Atlanta, GA
- ThP 629 **Analysis of Heavy Metals Using Porphyrin Decorated Hydrophobic Materials Coupled with MALDI-MS Measurement**; Hsin-You Tseng<sup>1</sup>; He-Hsuan Hsiao<sup>1</sup>; <sup>1</sup>Department of Chemistry, National Chung Hsing University, Taichung, Taiwan
- ThP 630 **C18-functionalized Manganese Ferrite Magnetic Nanoparticles in Combination with LDI-MS for the Analysis of Malachite Green**; Chang-En Lee<sup>1</sup>; He-Hsuan Hsiao<sup>1</sup>; <sup>1</sup>Department of Chemistry, National Chung Hsing University, Taichung, Taiwan
- ThP 631 **An Optimized MALDI Assay for Tree Gum Discrimination in Works of Art**; Katherine J Kenney<sup>1</sup>; Daniel D. Vallejo<sup>1</sup>; Katell Bathany<sup>2,3</sup>; Caroline Tokarski<sup>2,3</sup>; Facundo M. Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>University of Bordeaux, CNRS, Bordeaux INP, CBMN, UMR 5248, Pessac, France; <sup>3</sup>Bordeaux Proteome Platform, University of Bordeaux, Bordeaux, France
- ThP 632 **Building a database of membrane glycolipid barcodes using a rapid purification-free and target-agnostic MALDI-TOF MS lipid analysis technique**; Ian P. O'Keefe<sup>1</sup>; Linda Vu<sup>1</sup>; Moira Overly<sup>1</sup>; Hyojik Yang<sup>1</sup>; Richard D. Smith<sup>1</sup>; Matthew E. Sherman<sup>1</sup>; DAVID R GOODLETT<sup>2</sup>; Charles R. Sweet<sup>3</sup>; ROBERT K ERNST<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore, Baltimore, MD; <sup>2</sup>University of Victoria, Victoria, BC; <sup>3</sup>United States Naval Academy, Annapolis, MD
- ThP 633 **MALDI imaging of Drosera capensis indicates changes in abundance and spatial distribution of biomolecules after induced digestion**; Jonathan V. Le<sup>1</sup>; Zane G. Long<sup>1</sup>; Rachel W. Martin<sup>1</sup>; <sup>1</sup>University of California, Irvine, Irvine, CA
- ThP 634 **Interfacial Dynamics: Molecular Insights into Cacao Butter Phospholipids and their Influence on Water/Oil Emulsion Stability**; Luis M. Diaz-Sánchez<sup>1</sup>; Laura A.

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- Paiba<sup>1</sup>; Luis G. Gómez-Martínez<sup>2</sup>; Aldo F. Combariza<sup>2</sup>; Cristian Blanco-Tirado<sup>1</sup>; Marianny Y. Combariza<sup>1</sup>; <sup>1</sup>Universidad Industrial de Santander, Bucaramanga, Colombia; <sup>2</sup>Universidad de Sucre, Sincelejo, Colombia
- ThP 635 **Evaluating association of perfluorooctanesulfonic acid (PFOS) to bacteria using MALDI-MS;** Irfath Jasmin Reza<sup>1</sup>; Tian Autumn Qiu<sup>1, 2</sup>; <sup>1</sup>Michigan State University Department of Chemistry, East Lansing, MI; <sup>2</sup>MSU Center for PFAS Research, East Lansing, Michigan
- ThP 636 **Unraveling Phytoplankton Communities in a Marine Ecosystem through MALDI-FT-ICR Profiling;** Luis M. Díaz-Sánchez<sup>1</sup>; Martha L. Chacón-Patiño<sup>2</sup>; Chad R. Weisbrod<sup>2</sup>; Julián Franco<sup>3</sup>; Lizbeth J. Vivas-Aguas<sup>3</sup>; David Stranz<sup>4</sup>; Scott Campbell<sup>1</sup>; Cristian Blanco-Tirado<sup>1</sup>; Marianny Y. Combariza<sup>1</sup>; <sup>1</sup>Universidad Industrial de Santander, Bucaramanga, Colombia; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>Marine and Coastal Research Institute-INVEMAR, Santa Marta, Colombia; <sup>4</sup>Sierra Analytics, Modesto, California
- ThP 637 **AP/MALDI with high resolution and triple quadrupole mass analyzers for sensitive and high-throughput food authenticity analysis;** Nivedita Bhattacharya<sup>1, 2</sup>; Vishal Mahale<sup>1, 2</sup>; Madhuri Gupta<sup>1, 2</sup>; Nasiruddin Sheikh<sup>3</sup>; Akshay Vasekar<sup>3</sup>; Madhura Thete<sup>2</sup>; Enrico Davoli<sup>4</sup>; Kaushik Banerjee<sup>3</sup>; Venkateswarlu Panchagnula<sup>1, 2</sup>; <sup>1</sup>MassTech Inc., Columbia, MD; <sup>2</sup>Barefeet Analytics Pvt. Ltd., Pune, India; <sup>3</sup>ICAR-National Research Centre for Grapes, Manjiri Farm, P B, No 3, Solapur Rd, Pune, Maharashtra 412307, India, Pune, India; <sup>4</sup>Mario Negri Institute for Pharmacological Research, Via Mario Negri, 2, 20156 Milano MI, Italy, Europe, Milano, Italy
- ThP 638 **Advances in block copolymer materials research enabled by MALDI-TOF mass spectrometry;** Alyssa W. May<sup>1</sup>; Joseph G. Luther<sup>1</sup>; Travis S. Bailey<sup>1</sup>; <sup>1</sup>Colorado State University, Fort Collins, CO

### MALDI: INNOVATION IN INSTRUMENTATION AND SAMPLE PREPARATION 639-644

- ThP 639 **Burst Nucleation of Matrix on Doped Graphene for Quantitative MALDI-ToF Mass Spectrometry with Tunable Ion Yield;** Sanghwan Park<sup>1</sup>; Chang Young Lee<sup>1</sup>; <sup>1</sup>Ulsan National Institute of Science and Technology, Ulsan, South Korea
- ThP 640 **A Plug-and-Play Laser Post-Ionization Module for AP-MALDI-2 Orbitrap Mass Spectrometry Imaging with Improved Sensitivity;** Maureen Feucherolles<sup>1</sup>; Olivier Bouton<sup>2</sup>; Mathieu Gérard<sup>2</sup>; Eugene Moskovets<sup>3</sup>; Gilles Frache<sup>1</sup>; <sup>1</sup>Luxembourg Institute of Science and Technology, Molecular and Thermal Analysis, Belvaux, Luxembourg; <sup>2</sup>Luxembourg Institute of Science and Technology, Conception & prototyping, Belvaux, Luxembourg; <sup>3</sup>MassTech Inc., Columbia, MD
- ThP 641 **Centrifuge Tube Filters for Effective Bacterial Capture and Lysis from Biofluids for MALDI-based Mass Fingerprinting;** Austin R. Anderson<sup>1</sup>; Erick S. LeBrun<sup>1</sup>; Nileena Velappan<sup>1</sup>; Emilio S. Rivera<sup>1</sup>; Kes A. Luchini<sup>1</sup>; Ethan M. McBride<sup>2</sup>; Trevor G. Glaros<sup>1</sup>; <sup>1</sup>Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; <sup>2</sup>Los Alamos National Laboratory, Los Alamos, NM
- ThP 642 **Analysis of Small Biomolecules Aided by a Broad-Spectrum Reactive/Electron-Transfer Matrix; Covalent Radical Generating (CovRAGE) MALDI;** Cameron J. Kaminsky<sup>1</sup>; Hua Zhang<sup>2</sup>; Lingjun Li<sup>1, 2</sup>; <sup>1</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>School of Pharmacy, Madison, Wisconsin
- ThP 643 **Sample preparation method for fresh-frozen, undecalcified rat spine for MALDI MSI;** Kayle J. Bender<sup>1</sup>; Yongheng Wang<sup>2</sup>; Chuo Ying Zhai<sup>1</sup>; Zoe Saenz<sup>3</sup>; Aijun Wang<sup>4, 5</sup>; Elizabeth K. Neumann<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of California, Davis, Davis, California; <sup>2</sup>Department of Biomedical Engineering, University of California, Davis, California; <sup>3</sup>Department of Surgery, School

of Medicine, University of California, Davis, Sacramento, California; <sup>4</sup>Center for Surgical Bioengineering, Department of Surgery, School of Medicine, University of California, Davis, Sacramento, California; <sup>5</sup>Institute for Pediatric Regenerative Medicine, Shriners Hospital for Children Northern California, UC Davis School of Medicine, Sacramento, California

- ThP 644 **Exchange of Buffer System for MALDI-MS Analysis of Oligonucleotides without Desalting;** Andreas Baumeister<sup>1</sup>; Ido Bachelet<sup>2</sup>; Ronen Weiss<sup>2</sup>; <sup>1</sup>Shimadzu Europa GmbH, Duisburg, Germany; <sup>2</sup>Augmanity Nano Ltd, Rehovot, Israel

### METABOLOMICS: TARGETED AND QUANTITATIVE ANALYSIS II 645-666

- ThP 645 **Effects of Dietary Docosaheptaenoic Acid on Lipid Peroxidation Products in Mice Brain;** Kate Nyarko<sup>1</sup>; Michael Greenlief<sup>1</sup>; <sup>1</sup>University of Missouri-Columbia, Columbia, MO
- ThP 646 **Establishing an energy-related metabolism platform using cyanopropyl-based LC-MS/MS;** Wan-Rou Liao<sup>1</sup>; Sung-Fang Chen<sup>2</sup>; <sup>1</sup>National Taiwan Normal University, Taipei, Taiwan; <sup>2</sup>National Taiwan Normal University, Taipei, Taiwan
- ThP 647 **Quantification of Cyanogenic Glycosides using LC-MS/MS MRM;** Zhentian Lei<sup>1</sup>; Deepak Kasote<sup>1</sup>; Clayton D. Kranawetter<sup>1</sup>; Ashley C. Conway-Anderson<sup>1</sup>; Barbara W. Sumner<sup>1</sup>; Lloyd W. Sumner<sup>1</sup>; <sup>1</sup>University of Missouri, Columbia, MO
- ThP 648 **Quantitative and qualitative analysis of steroids by high-resolution mass spectrometry;** Robert Proos<sup>1</sup>; Paul RS Baker<sup>1</sup>; Nicole Abbott<sup>2</sup>; Kasey Hill<sup>2</sup>; Mitch A. Phelps<sup>2</sup>; <sup>1</sup>Sciex, Framingham, MA; <sup>2</sup>Ohio State University, Columbus, OH
- ThP 649 **Determination of Plasma Free Amino Acids in Biological Samples using Liquid Chromatography-Tandem Mass Spectrometry;** Jaeman Byun<sup>1</sup>; Subramanian Pennathur<sup>1</sup>; Anna Mathew<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI
- ThP 650 **High-resolution Quantitative Metabolomics with biocrates' AbsoluteIDQ® p400 HR kit on Thermo Scientific™ Orbitrap Exploris™ Hybrid Mass Spectrometry Platforms;** Guohui Li<sup>1</sup>; Stephen Dearth<sup>2</sup>; Joshua P. Kline<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific – 355 River Oaks Pkwy, San Jose, California; <sup>2</sup>biocrates life sciences ag – Eduard-Bodem-Gasse 8, Innsbruck, Austria
- ThP 651 **Metabolomics Changes Associated with the Development and Progression of Parkinson's Disease Identified Through Parallel Reaction Monitoring LC-MS/MS;** Oduwayo O. Oluokun<sup>1</sup>; Oluwatosin E. Daramola<sup>1</sup>; Judith Nwaiwu<sup>1</sup>; Mojibola Fowowe<sup>1</sup>; Andrew I. Bennett<sup>1</sup>; Alexandra Lux<sup>1</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX
- ThP 652 **Targeted Metabolomic Analysis: Discriminating Hybrid and Wild Hippastrum Species (Amaryllidaceae) through Alkaloid Profiling by LC-ESI(±)LTQ MS;** Amanda Eiriz Feu<sup>1</sup>; Marcos Valério Vieira Lyrio<sup>1</sup>; Wanderson Romão<sup>1</sup>; Warley de Souza Borges<sup>1</sup>; <sup>1</sup>UFES, Vitória, Brazil
- ThP 653 **Direct comparison of a machine learning-based tool for rapid absolute quantification of metabolites in biological samples with traditional isotopologue analysis;** Ana S. H. Costa<sup>1</sup>; Craig Knisley<sup>1</sup>; Timothy Kassis<sup>1</sup>; Mimoun Cadosch Delmar<sup>1</sup>; Lucas Reger<sup>2</sup>; Julia Niemann<sup>2</sup>; David Pollard<sup>2</sup>; Joshua D. Lauterbach<sup>1</sup>; Luke S. Ferro<sup>1</sup>; Steven B. Hooper<sup>1</sup>; Jack Howland<sup>1</sup>; Jefferson G. Pruyne<sup>1</sup>; Jennifer M. Campbell<sup>1</sup>; Jack Geremia<sup>1</sup>; <sup>1</sup>Matterworks, Inc., Somerville, MA; <sup>2</sup>Sartorius Stedim Biotech GmbH, Goettingen, Germany
- ThP 654 **Pushing the boundaries of speed in Metabolomics: coupling microfluidic capillary electrophoresis with the new ultrafast hybrid nominal mass instrument;** Cristina C. Jacob<sup>1</sup>; Charles Maxey<sup>1</sup>; Philip M. Remes<sup>1</sup>; J. Will Thompson<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>908 Devics Inc., Morrisville, NC
- ThP 655 **A fast and robust LC-MS method for the analysis of basal metabolism in multiple mammalian tissues;** Haiyan Ke<sup>1, 2</sup>; Poonamjot Deol<sup>1</sup>; Manhoi Hur<sup>1, 2</sup>; John Leano<sup>1</sup>; Frances

## THURSDAY POSTERS

- Sladek<sup>1</sup>; Amancio J De Souza<sup>1,2</sup>; <sup>1</sup>University of California Riverside, Riverside, CA; <sup>2</sup>UCR Metabolomics Core, University of California, Riverside, California
- ThP 656 **Identification and quantification of cyclic dipeptides in human serum using mass spectrometry**; Anthony Haag<sup>1</sup>; Kathleen Hoch<sup>1</sup>; Sigmund Haidacher<sup>1</sup>; Nian Liu<sup>1</sup>; Tor Savidge<sup>1</sup>; <sup>1</sup>Baylor College of Medicine, Houston, Texas
- ThP 657 **Intra-laboratory validation of four LC/MS quantitative analytical methods for human plasma metabolomics data integration**; Yuri Imado<sup>1</sup>; Masatomo Takahashi<sup>1,2</sup>; Yuki Soma<sup>3</sup>; Kohta Nakatani<sup>1,2</sup>; Taizo Hanai<sup>3</sup>; Yoshihiro Izumi<sup>1,2</sup>; Takeshi Bamba<sup>1,2</sup>; <sup>1</sup>Graduate School of Systems Life Sciences, Kyushu University, Fukuoka, Japan; <sup>2</sup>Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; <sup>3</sup>Graduate School of Bioresource and Bioenvironmental Sciences, Kyushu University, Fukuoka, Japan
- ThP 658 **International ring trial of a standardized quantitative assay analyzing more than 1,000 metabolites across eleven laboratories and seven LC-MS platforms**; Markus Langsdorf<sup>1</sup>; Gregor Ömer<sup>1</sup>; Cornelia Röhring<sup>1</sup>; Tuan Hai Pham<sup>1</sup>; <sup>1</sup>biocrates life sciences ag, Innsbruck, Austria
- ThP 659 **Urinary metabolomics profiling across mass spectrometer platforms using optimized, matrix-specific calibration standards, quality controls, and acquisition methods**; Gregor Ömer<sup>1</sup>; Markus Langsdorf<sup>1</sup>; Stephen Dearth<sup>1</sup>; <sup>1</sup>biocrates life sciences ag, Innsbruck, Austria
- ThP 660 **Short Chain Fatty Acid Quantification: Standard Curve or Ratio Quantification?**; Aryeh Korman<sup>1</sup>; Rebecca Jones<sup>1</sup>; Supinda Bunyavanich<sup>2</sup>; Drew R. Jones<sup>1</sup>; <sup>1</sup>NYU Langone, New York, NY; <sup>2</sup>Icahn School of Medicine at Mount Sinai, New York, NY
- ThP 661 **Towards the understanding of lactate accumulation with CHO cell culture metabolite profiling**; Bo Zhai<sup>1</sup>; Elsa Gorre<sup>1</sup>; Kathryn Dorst<sup>1</sup>; Christopher Sauer<sup>1</sup>; Hirsh Nanda<sup>1</sup>; <sup>1</sup>Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania
- ThP 662 **Quantification of intra- and extracellular metabolites in Birt-Hogg-Dubé syndrome renal tumors by Ultra-High-Resolution Mass Spectrometry based Stable-Isotope-Resolved Metabolomics**; Ye Yang<sup>1</sup>; Daniel Crooks<sup>1</sup>; Laura S. Schmidt<sup>1,2</sup>; Christopher J. Ricketts<sup>1</sup>; Nunziata Maio<sup>3</sup>; Ronald Holewinski<sup>4</sup>; Thorkell Andresson<sup>4</sup>; Richard Higashi<sup>5</sup>; Teresa W.-M. Fan<sup>5</sup>; Andrew Lane<sup>5</sup>; Youfeng Yang<sup>1</sup>; Cathy C. Vocke<sup>1</sup>; W. Marston Linehan<sup>1</sup>; <sup>1</sup>Urologic Oncology Branch, Center for Cancer Research, National Cancer Institute, National Institutes of Health, Bethesda, MD; <sup>2</sup>Basic Science Program, Frederick National Laboratory for Cancer Research, National Cancer Institute, Frederick, MD; <sup>3</sup>Section on Cell Biology and Metabolism, Eunice Kennedy Shriver National Institute of Child Health and Human Development, National Institutes of Health, Bethesda, MD; <sup>4</sup>Leidos Biomedical Research, Inc., Frederick National Laboratory for Cancer Research, National Cancer Institute, Bethesda, MD; <sup>5</sup>Department of Toxicology and Cancer Biology, Markey Cancer Center, University of Kentucky, Lexington, KY
- ThP 663 **Efficient and Improved LC-MS/MS Quantitation of Phenolic Acids and Lignans from Human Fecal Samples**; Chris Dickson<sup>1</sup>; Jonathan Rickmeyer<sup>2</sup>; Felix Grun<sup>2</sup>; Elizabeth Bess<sup>2</sup>; <sup>1</sup>University of California Irvine, Irvine, CA; <sup>2</sup>University of California, Irvine, Irvine, CA
- ThP 664 **In vivostable isotope tracing and metabolomics for the identification of synthetically lethal metabolic vulnerabilities in glioblastomas**; Suresh Udutha<sup>1</sup>; Céline Taglang<sup>1</sup>; Georgios Batsios<sup>1</sup>; Anne Marie Gillespie<sup>1</sup>; Meryssa Tran<sup>1</sup>; Pavithra Viswanath<sup>1</sup>; <sup>1</sup>UCSF, San Francisco, CA
- ThP 665 **Development of a Simultaneous Quantitation and Discovery (SQUAD) workflow for coeluting sugar-phosphates using orthogonal fragmentation techniques**; Sunandini Yedla<sup>1</sup>; Brandon Bills<sup>1</sup>; Rahul Deshpande<sup>1</sup>; Bashar Amer<sup>1</sup>; Susan S Bird<sup>1</sup>; Vlad Zabrouskov<sup>1</sup>; <sup>1</sup>ThermoFisher Scientific, San Jose, CA
- ThP 666 **Development and Evaluation of a Fast LC-MS Assay to Quantify NAD-Associated Metabolites in Cancer Cells**; Mike Lingue Wang<sup>1</sup>; Ryan Conrad<sup>1</sup>; Scott Foster<sup>1</sup>; Dewakar Sangaraju<sup>1</sup>; Xiaorong Liang<sup>1</sup>; Brian Dean<sup>1</sup>; Zijuan Lai<sup>1</sup>; <sup>1</sup>Genentech Inc., South San Francisco, CA

### NATURAL PRODUCTS 667-694

- ThP 667 **The membrane protein Rv2113 is crucial for the anti-tubercular activity of Callyaerins**; David Podlesainski<sup>1</sup>; Emmanuel Tola Adeniyi<sup>2</sup>; Violetta Krisilia<sup>2</sup>; Florian Schulz<sup>1</sup>; Tim Richter<sup>1</sup>; Farnusch Kaschani<sup>1</sup>; Rainer Kalscheuer<sup>2</sup>; Markus Kaiser<sup>1</sup>; <sup>1</sup>University Duisburg-Essen, Essen, Germany; <sup>2</sup>Heinrich Heine University, Düsseldorf, Germany
- ThP 668 **Rationally Minimizing Natural Product Libraries without Chemical Diversity Sacrifice using Untargeted Metabolomics**; Monica Ness<sup>1,2</sup>; Thilini Peramuna<sup>1</sup>; Karen Wendt<sup>1</sup>; Crystal Okeke<sup>1</sup>; Robert H Cichewicz<sup>1</sup>; Laura-Isobel McCall<sup>1,2</sup>; <sup>1</sup>University of Oklahoma, Norman, OK; <sup>2</sup>San Diego State University, San Diego, CA
- ThP 669 **Comparing the attachment disc composition of aquatic, diving bell spiders to terrestrial black widow spiders using SL-MALDI-MSI and MALDI-MS/MS**; Calum Bochenek<sup>1</sup>; Bernd Stekli<sup>1</sup>; Tyler Arntz<sup>1</sup>; Todd Blackledge<sup>1</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>The University of Akron, Akron, OH
- ThP 670 **Bridging the Gap: A Comparative Analysis of Orbitrap and Ion Cyclotron Resonance Mass Spectrometers on Natural Organic Matter**; Charlotte Brun<sup>1</sup>; Mourad Hari<sup>2</sup>; Christos Panagiotopoulos<sup>3</sup>; Philippe Schmitt-Kopplin<sup>2,4</sup>; Sébastien Schramm<sup>5</sup>; Maxime Bridoux<sup>1</sup>; <sup>1</sup>CEA, DAM, DIF, F-91297, Arpajon, France; <sup>2</sup>Research Unit Analytical BioGeoChemistry, Helmholtz Munich, 85764 Neuherberg, Germany; <sup>3</sup>M.I.O. Institut Méditerranéen d'Océanologie, Aix Marseille Univ., Université de Toulon, CNRS, IRD, F-13288, Marseille, France; <sup>4</sup>Analytical Food Chemistry, TUM, Maximus-von-Imhof-Forum 2, 85354 Freising, Germany; <sup>5</sup>Laboratoire de Chimie et de Physique – Approches Multi-échelles des Milieux Complexes (LCP-A2MC), Université de Lorraine, F-57078, Metz, France
- ThP 671 **Influence of Geographic Variation on Chemistry and Metabolomics of Pacific Northwest Endemic Lobaria sp. Cyanolichens**; Xinhui Yu<sup>1</sup>; Wilmer Perera<sup>2</sup>; Joseph Di Meglio<sup>3</sup>; Bruce McCune<sup>3</sup>; Kerry McPhail<sup>3</sup>; <sup>1</sup>Oregon State University, Corvallis, OR; <sup>2</sup>CAMAG Scientific, Wilmington, NC; <sup>3</sup>Oregon State University, Corvallis, Oregon
- ThP 672 **In-depth characterization and structure elucidation of non-ribosomal peptides related to adenopeptin using LC-HRAM-MSn**; Douglas Marchbank<sup>1</sup>; Sven Hackbusch<sup>2</sup>; Bradley Hattli<sup>1</sup>; Brandon Bills<sup>3</sup>; Min Du<sup>4</sup>; <sup>1</sup>Croda Canada Ltd, Charlottetown, PEI; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>ThermoFisher Scientific, San Jose, CA; <sup>4</sup>Thermo Fisher Scientific, Lexington, MA
- ThP 673 **Identification of antimicrobial peptides against bacterium Burkholderia glumae**; Jeffrey Ocampo<sup>1</sup>; Leslie M. Hicks<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC
- ThP 674 **Investigation of the Underlying Mechanism of Lasso Peptide Thermal Unthreading using LC-TIMS-q-ECD ToF MS/MS**; Kevin Jeanne Dit Fouque<sup>1</sup>; Miguel Santos<sup>1</sup>; Negin Asgharihosseinpour<sup>2</sup>; Severine Zirah<sup>3</sup>; Julian D Hegemann<sup>2</sup>; Francisco A Fernandez-Lima<sup>1</sup>; <sup>1</sup>Florida International University, Miami, FL; <sup>2</sup>Saarland University, Saarbrücken, Germany; <sup>3</sup>National Museum of Natural History, Paris, France
- ThP 675 **Induction of Plant Bioactive Peptides in Response to Environmental Stressors**; Katelyn D Wix<sup>1</sup>; Leslie M. Hicks<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC
- ThP 676 **Characterization of the lasso and branched-cyclic Cyanodin I using Hydrogen-Deuterium Exchange, Trapped Ion Mobility Spectrometry, and tandem ECD-MS/MS**; Miguel Santos<sup>1</sup>; Kevin Jeanne Dit Fouque<sup>1</sup>; Ukesh Karki<sup>1</sup>; Julian D Hegemann<sup>2</sup>; Prem Chapagain<sup>1</sup>; Francisco A Fernandez-Lima<sup>1</sup>; <sup>1</sup>Florida International University, Miami, FL; <sup>2</sup>Helmholtz Institute for Pharmaceutical Research

## THURSDAY POSTERS

- Saarland (HIPS), Helmholtz Centre for Infection Research, Saarbrücken, Germany
- ThP 677 **Assessing biological and metabolic diversity in Trichoderma for natural product library assembly using untargeted metabolomics**; Thilini Peramuna<sup>1</sup>; Monica Ness<sup>1,2</sup>; Karen Wendt<sup>1</sup>; Robert H Cichewicz<sup>1</sup>; Laura-Isobel McCall<sup>2</sup>; <sup>1</sup>University of Oklahoma, Norman, OK; <sup>2</sup>San Diego State University, San Diego, CA
- ThP 678 **Determination of cycloastragenol in dietary supplements containing the adaptogenic herb Astragalus trimestris using HPLC-MS/MS**; Katerina Knizkova<sup>1</sup>; Martin Kuchar<sup>1</sup>; Petra Cihlarova<sup>1</sup>; <sup>1</sup>Forensic Laboratory of Biologically Active Substances, Department of Chemistry of Natural Compounds, University of Chemistry and Technology, Prague, Czech Republic
- ThP 679 **Determination of 2-phenoxychromones and structurally related flavonols using LC-QTOF tandem mass spectrometry combined with molecular networking analysis**; In Jin Ha<sup>1,2</sup>; Min Young Lee<sup>1</sup>; Seok-Geun Lee<sup>1,2</sup>; Kwang Seok Ahn<sup>2</sup>; Junhee Lee<sup>1,2</sup>; <sup>1</sup>Kyung Hee University Korean Medicine Hospital, Seoul, South Korea; <sup>2</sup>College of Korean Medicine, Kyung Hee University, Seoul, South Korea
- ThP 680 **A rapid method to differentiate and identify isomers of A-type procyanidins**; Pai-Chi Syue<sup>1</sup>; Kuok Fai Li<sup>1</sup>; Kuo-Lung Ku<sup>1</sup>; Yao-Yuan Chuang<sup>2</sup>; <sup>1</sup>National Chiayi University, Chiayi City, Taiwan; <sup>2</sup>National University of Kaohsiung, Kaohsiung City, Taiwan
- ThP 681 **Detection of Upregulation and Downregulation of Fungal Secondary Metabolism from Penicillium spp by Liquid Microjunction Surface Sampling Probe (LMJSSP)**; Jessie F. Deng<sup>1</sup>; Jennifer L. Kolwich<sup>1</sup>; Haidy Metwally<sup>1</sup>; Georgia Reed<sup>2</sup>; Randy E. Ellis<sup>2,3,4,5</sup>; Avena C. Ross<sup>1</sup>; Richard D. Oleschuk<sup>1</sup>; <sup>1</sup>Department of Chemistry, Queen's University, Kingston, ON; <sup>2</sup>School of Computing, Queen's University, Kingston, ON; <sup>3</sup>Department of Mechanical and Materials Engineering, Queen's University, Kingston, ON; <sup>4</sup>Department of Surgery, Queen's University, Kingston, ON; <sup>5</sup>Department of Biomedical and Molecular Sciences, Queen's University, Kingston, ON
- ThP 682 **Mapping Metabolite Dynamics of Soil Microbe Interactions using a Liquid Microjunction Surface Sampling Probe (LMJSSP)**; Jennifer L. Kolwich<sup>1</sup>; Lainey K. Ennett<sup>1</sup>; Jessie F. Deng<sup>1</sup>; Richard D. Oleschuk<sup>1</sup>; Avena C. Ross<sup>1</sup>; <sup>1</sup>Queen's University, Kingston, ON
- ThP 683 **UHPLC-MS/MS profiling of alkaloids in opium and poppy straw**; Petra Cihlarova<sup>1</sup>; Viktorie Lukesova<sup>1</sup>; Katerina Knizkova<sup>1</sup>; Martin Kuchar<sup>1</sup>; <sup>1</sup>Forensic Laboratory of Biologically Active Substances, Department of Chemistry of Natural Compounds, University of Chemistry and Technology, Prague, Czech Republic
- ThP 684 **Use of IMS HDMSe for the Analysis of Anthocyanins, Procyanidins and Other Flavonoids in Food and Natural Product Samples**; Gordon T Fujimoto<sup>1</sup>; Lindsay E Hatch<sup>1</sup>; Sarah E Dowd<sup>1</sup>; Emily R Britton<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, Massachusetts
- ThP 685 **Development of a novel non-targeted method for authentication of American ginseng using ASAP-MS and UPLC-QTOF-MS**; Sanem Hosbas Coskun<sup>1,2</sup>; Aaron A. Urbas<sup>2</sup>; Adam J. Kuszak<sup>1</sup>; Aysel Berkan<sup>2,3</sup>; Benjamin J. Place<sup>2</sup>; Catherine A. Rimmer<sup>2</sup>; David A. Sheen<sup>2</sup>; <sup>1</sup>Office of Dietary Supplements, National Institutes of Health, Bethesda, MD; <sup>2</sup>National Institute of Standards and Technology, Gaithersburg, MD; <sup>3</sup>Gazi University Faculty of Pharmacy Department of Analytical Chemistry, Ankara, Turkey
- ThP 686 **Knowledge-based data strategies bridge the gap for automated data analysis of phytochemical diversity in Withania somnifera**; Rudranil Dutta<sup>1,2</sup>; Luke C Marney<sup>1,2</sup>; Jaewoo Choi<sup>1,2</sup>; Liping Yang<sup>1,2</sup>; Amala Soumyanath<sup>2,3</sup>; Jan F. Stevens<sup>2,4,5</sup>; Claudia S. Maier<sup>1,2,4</sup>; <sup>1</sup>Department of Chemistry, Oregon State University, Corvallis, OR; <sup>2</sup>BENFRA Botanical Dietary Supplements Research Center, Oregon Health and Science University, Portland, OR;
- <sup>3</sup>Department of Neurology, Oregon Health and Science University, Portland, Oregon; <sup>4</sup>Linus Pauling Institute, Oregon State University, Corvallis, OR; <sup>5</sup>Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR
- ThP 687 **Mass Spectrometric Analysis of Antifungal Secondary Metabolites of a Streptomyces murinus Isolate from Vietnam**; Cloe R Zimmerman<sup>1,2</sup>; Thi Thuy Tien Nguyen<sup>3</sup>; Lauren Konig<sup>1,4</sup>; Karine Bagramyan<sup>1</sup>; Markus Kalkum<sup>1,2</sup>; <sup>1</sup>Department of Immunology and Theranostics, City of Hope, Duarte, CA; <sup>2</sup>Irell & Manella Graduate School of Biological Sciences, City of Hope, Duarte, CA; <sup>3</sup>Department of Engineering and Food Technology, University of Agriculture and Forestry, Hue University, Hue City, Vietnam; <sup>4</sup>Indiana University Bloomington, Bloomington, IN
- ThP 688 **Discovering bioactive compounds in Centella asiatica by chromatographic fractionation, flow-injection ion-mobility mass spectrometry, ARE/NRF2 response, and ensemble elastic net regression**; Luke C Marney<sup>1,2</sup>; Vera Alenicheva<sup>1,2</sup>; Bailey Keefe<sup>3</sup>; Jaewoo Choi<sup>1,2</sup>; Liping Yang<sup>1,2</sup>; Nora Gray<sup>2,4</sup>; Amala Soumyanath<sup>2,4</sup>; Kevin Brown<sup>2,3,5</sup>; Jan F. Stevens<sup>2,3,6</sup>; Claudia S. Maier<sup>1,2,6</sup>; <sup>1</sup>Department of Chemistry, Oregon State University, Corvallis, OR; <sup>2</sup>BENFRA Botanical Dietary Supplements Research Center, Oregon Health and Science University, Portland, OR; <sup>3</sup>Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR; <sup>4</sup>Department of Neurology, Oregon Health and Science University, Portland, Oregon; <sup>5</sup>School of Chemical, Biological, and Environmental Engineering, Oregon State University, Corvallis, Oregon; <sup>6</sup>Linus Pauling Institute, Oregon State University, Corvallis, OR
- ThP 689 **HRAM analysis and spectral data mining of museum-sourced cnidarian extracts for natural product investigations**; Jennifer E Netjes<sup>1</sup>; Sam Afoullouss<sup>1</sup>; Dale Chaput<sup>1</sup>; Andrea Quattrini<sup>2</sup>; Bill Baker<sup>1</sup>; <sup>1</sup>University of South Florida, Tampa, FL; <sup>2</sup>National Museum of Natural History, Smithsonian Institution, Washington, DC
- ThP 690 **Molecular network guided isolation of new aphrocallistin for deep-sea sponge Aphrocallistes sp enhanced by Ion Mobility**; Sam Afoullouss<sup>1</sup>; Jennifer Netjes<sup>1</sup>; Ryan M. Young<sup>2</sup>; Fred Valeriotte<sup>3</sup>; Mark P. Johnson<sup>2</sup>; A. Louise Allcock<sup>2</sup>; Bill J. Baker<sup>1</sup>; <sup>1</sup>University of South Florida, Tampa, FL; <sup>2</sup>Ryan Institute & School of Natural Sciences, University of Galway, University Road, Galway, Ireland, Galway, Ireland; <sup>3</sup>Department of Internal Medicine, Division of Hematology and Oncology, Henry Ford Hospital, Detroit, MI
- ThP 691 **Comparison of nocturnal and diurnal metabolomes of rose flowers and leaves**; Julie Zumsteg<sup>1</sup>; Elodie Bossard<sup>2</sup>; Lorène Gourguillon<sup>2</sup>; Claire Villette<sup>1</sup>; Dimitri Heintz<sup>1</sup>; <sup>1</sup>CNRS IBMP, Strasbourg, France; <sup>2</sup>Advanced Biobased and Bioinspired Ingredients, LVMH Recherche, Saint-Jean-de-Braye, France
- ThP 692 **Towards the isolation of traditionally utilized plant-origin antiparasitic compounds through chemometrics-guided serial fractionation and in vitro assay**; Grace Ochigbo<sup>1</sup>; Brenda Holder<sup>2</sup>; Ralph Hindle<sup>3</sup>; Kathy Hunt<sup>3</sup>; James D Wasmuth<sup>1</sup>; Brielle V Rosa<sup>1</sup>; <sup>1</sup>University of Calgary, Faculty of Veterinary Medicine, Calgary, AB; <sup>2</sup>Cree Traditional Knowledge Keeper, Jasper National Park, AB; <sup>3</sup>Vogon Laboratory Services Ltd., Cochrane, AB
- ThP 693 **Comparison of Dried Thyme from Different Geographical Locations with GC-TOFMS and Software Tools Designed to Rapidly Determine Similarities and Differences**; Elizabeth M Humston-Fulmer<sup>1</sup>; David E Alonso<sup>1</sup>; John Hayes<sup>1</sup>; Joseph E Binkley<sup>1</sup>; <sup>1</sup>LECO Corporation, Saint Joseph, MI
- ThP 694 **Automation of QuEChERS extraction for quantitation of CBD and THC in cannabis leaves in 8 seconds per sample**; Jonathan Rochon<sup>1</sup>; Serge Auger<sup>1</sup>; Mégane Moreau<sup>1</sup>; Sarah Demers<sup>1</sup>; Jean Lacoursière<sup>1</sup>; Pierre Picard<sup>1</sup>; <sup>1</sup>Phytrox Technologies, Inc., Quebec, QC

THURSDAY POSTERS

695-715

- ThP 695 **Discovery of omega-3 polyunsaturated fat-derived lysine iminylation as a novel, chemically labile post-translational modification;** Bingsen Zhang<sup>1, 2</sup>; Frank C Schroeder<sup>1, 2</sup>; <sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>Boyce Thompson Institute, Ithaca, NY
- ThP 696 **Capturing the polyUbiquitylome with pUb-STRACTER (Stringent Trypsin-Resistant Affinity Capture with Targeted Enzymatic Recovery);** Harvey E. Johnston<sup>1</sup>; Rahul S. Samant<sup>1</sup>; <sup>1</sup>Babraham Institute, Cambridge, United Kingdom
- ThP 697 **Re-exploring Zirconia Chromatography to Enhance Phosphoproteome Coverage;** Kosuke Ogata<sup>1</sup>; Naoyuki Sugiyama<sup>1</sup>; Yasushi Ishihama<sup>1, 2</sup>; <sup>1</sup>Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; <sup>2</sup>National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan
- ThP 698 **-Exploring the role of reversible cysteine oxidation in tardigrade osmobiogenesis;** Samantha J Balboa<sup>1</sup>; Evan R. Stair<sup>1</sup>; Meredith H. Daughtridge<sup>1</sup>; Abel A. Salas<sup>1</sup>; Brendin Flinn<sup>2</sup>; Derrick Kolling<sup>2</sup>; Leslie M. Hicks<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>2</sup>Marshall University, Huntington, West Virginia
- ThP 699 **Comprehensive characterization of biotherapeutics using orthogonal capillary electrophoresis (CE), liquid chromatography-mass spectrometry (LC-MS) and imaged capillary isoelectric focusing (icIEF)-UV/MS workflows;** Zoe Zhang<sup>1</sup>; Haichuan Liu<sup>2</sup>; Marcia Santos<sup>3</sup>; Rashmi Madda<sup>2</sup>; Jingwen Ding<sup>4</sup>; Scott Mack<sup>4</sup>; Maggie Ostrowski<sup>4</sup>; Elliott Jones<sup>2</sup>; Paul Clemens<sup>2</sup>; <sup>1</sup>Sciex, Redwood City, CA; <sup>2</sup>SCIEX, Redwood City, CA; <sup>3</sup>SCIEX, Brea, CA; <sup>4</sup>SCIEX, Fremont, CA
- ThP 700 **Short-chain fatty acids propionate and butyrate control growth and differentiation linked to cellular metabolism;** Michael Nshanian<sup>1</sup>; Benjamin S. Geller<sup>1</sup>; Joshua J. Gruber<sup>1</sup>; Faye Chleilat<sup>1</sup>; Jeannie Marie Camarillo<sup>2</sup>; Neil L. Kelleher<sup>2, 3</sup>; Yingming Zhao<sup>4</sup>; Michael P. Snyder<sup>1, 5</sup>; <sup>1</sup>Department of Genetics, Stanford University School of Medicine, Stanford, CA; <sup>2</sup>Department of Chemistry, Molecular Biosciences and Proteomics Center of Excellence, Northwestern University, Evanston, IL; <sup>3</sup>Department of Biochemistry and Molecular Genetics, Feinberg School of Medicine, Northwestern University, Evanston, IL; <sup>4</sup>Ben May Department of Cancer Research Committee on Cancer Biology, University of Chicago, Chicago, IL; <sup>5</sup>Center for Genomics and Personalized Medicine, Stanford University School of Medicine, Stanford, CA
- ThP 701 **DISCOVERY OF A NOVEL ITACONATE-MEDIATED METHYLSUCCINYLTATION;** Dongyang Liu<sup>1</sup>; Chu Wang<sup>1</sup>; <sup>1</sup>Peking University, Beijing, China
- ThP 702 **Methionine alkylation as an approach to quantify methionine oxidation using mass spectrometry;** Margaret M Hoare<sup>1</sup>; Ruiyue Tan<sup>1</sup>; Kevin A Welle<sup>2</sup>; Kyle Swovick<sup>2</sup>; Jennifer R Hryhorenko<sup>2</sup>; Sina Ghaemmaghami<sup>1, 2</sup>; <sup>1</sup>University of Rochester, Rochester, NY; <sup>2</sup>University of Rochester Mass Spectrometry Resource Laboratory, Rochester, NY
- ThP 703 **Investigating the self-pupylation of PafA in the Pup-proteasome system;** Jacquelyn C Ogata-Bean<sup>1</sup>; Alicia Plourde<sup>1</sup>; Siavash Vahidi<sup>1</sup>; <sup>1</sup>University of Guelph, Guelph, ON
- ThP 704 **Genotype-dependent N-glycosylation and novel O-glycosylation affect the activation of histidine-rich glycoprotein by plasmin;** Yang Zou<sup>1, 2</sup>; Matti F. Pronker<sup>1, 2</sup>; Karli R. Reiding<sup>1, 2</sup>; Albert J.R. Heck<sup>1, 2</sup>; <sup>1</sup>Utrecht University, Utrecht, Netherlands; <sup>2</sup>Netherlands Proteomics Center, Utrecht, Netherlands
- ThP 705 **Quantification of ADP-ribosylated proteins in neutrophils using an Orbitrap Astral mass spectrometer;** Hayoung Cho<sup>1</sup>; Ivo A Hendriks<sup>1</sup>; Michael L Nielsen<sup>1</sup>; <sup>1</sup>Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark
- ThP 706 **Multiplexed ubiquitome profiling in dozens of cell levels without enrichment using a boosting channel;** Minsang Hwang<sup>1, 2</sup>; Jong-Seo Kim<sup>1, 2</sup>; <sup>1</sup>School of Biological Sciences, Seoul National University, Seoul, South Korea; <sup>2</sup>Center for RNA Research, Institute of Basic Science (IBS), Seoul, South Korea
- ThP 707 **Site-Specific ADP-ribosylome Analysis Reveals Homogeneous DNA Damage-Induced Serine ADP-Ribosylation in Wild-Type and BRCA-Mutant Breast Cancer Cells;** Holda A Anagho<sup>1</sup>; Meeli Mullari<sup>1</sup>; Hayoung Cho<sup>1</sup>; Aurél G. Prósz<sup>2</sup>; Sara C. Buch-Larsen<sup>1</sup>; Marie Locard-Paulet<sup>3</sup>; Zoltan Szallasi<sup>2, 4</sup>; Michael L Nielsen<sup>1</sup>; <sup>1</sup>Novo Nordisk Foundation Center for Protein Research, Proteomics Program, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; <sup>2</sup>Danish Cancer Institute, Copenhagen, Denmark; <sup>3</sup>Institut de Pharmacologie et de Biologie Structurale (IPBS), Université de Toulouse, CNRS, Université Toulouse III - Paul Sabatier (UT3), Toulouse, France; <sup>4</sup>Computational Health Informatics Program, Boston Children's Hospital, Boston, MA
- ThP 708 **Optimal Dissociation Methods for Enhancing Identification and Quantitative Accuracy of Various Glycan Types in Intact N-glycopeptides Analysis;** Zhenyu Sun<sup>1</sup>; Yingwei Hu<sup>1</sup>; T. Mamie Lih<sup>1</sup>; Jongmin Woo<sup>1</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- ThP 709 **Bottom-Up, Middle-Down, or Top-Down Collision Induced Dissociation? Pros and Cons for Retaining and Localizing Labile Post-Translational Modifications;** Neven N. Mikawy<sup>1</sup>; Kristina Hakansson<sup>1</sup>; <sup>1</sup>University of Michigan Department of Chemistry, Ann Arbor, MI
- ThP 710 **Profiling Protein Post-Translational Modifications in Plasma-derived Extracellular Vesicles as Fingerprints for Breast Cancer Subtypes;** Marco Hadisurya<sup>1</sup>; Hillary Andaluz Aguilar<sup>2</sup>; Mengting Xu<sup>3</sup>; I-Hsuan Chen<sup>1</sup>; J. Sebastian Paez<sup>4</sup>; Zheng-Chi Lee<sup>1, 5</sup>; Anton B. Iliuk<sup>6</sup>; Sonia Sugg<sup>7</sup>; Weizhou Zhang<sup>8</sup>; W. Andy Tao<sup>1, 2, 4, 9</sup>; <sup>1</sup>Department of Biochemistry, Purdue University, West Lafayette, IN; <sup>2</sup>Department of Chemistry, Purdue University, West Lafayette, IN; <sup>3</sup>School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN; <sup>4</sup>Department of Medical Chemistry and Molecular Pharmacology, Purdue University, West Lafayette, IN; <sup>5</sup>West Lafayette Junior/Senior High School, West Lafayette, IN; <sup>6</sup>Tymora Analytical Operations, West Lafayette, IN; <sup>7</sup>College of Medicine, University of Iowa, Iowa City, IA; <sup>8</sup>College of Medicine, University of Florida, Gainesville, FL; <sup>9</sup>Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN
- ThP 711 **Identification of isoaspartic acid residues in proteins by deuterium labeling and mass spectrometry;** Masaru Miyagi<sup>1</sup>; Kelao Neumbo<sup>2</sup>; Takashi Nakazawa<sup>3</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>Case Western Reserve University, Cleveland, OH; <sup>3</sup>Nara Women's University, Nara, Japan
- ThP 712 **A Systematic Investigation of Citrullination and Corresponding Structural Effect in Human Rheumatoid Arthritis;** Zexin Zhu<sup>1</sup>; Wei Li<sup>2</sup>; Hung-Yu (Eric) Chiang<sup>3</sup>; Hua Zhang<sup>2</sup>; Zhicheng Jin<sup>4</sup>; Lingjun Li<sup>2</sup>; <sup>1</sup>University of Wisconsin - Madison, Madison, WI; <sup>2</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>Department of Biophysics, University of Wisconsin-Madison, Madison, WI; <sup>4</sup>Department of Pathology and Laboratory Medicine, University of Wisconsin-Madison, Madison, WI
- ThP 713 **Acetylation of RORβ DNA binding domain and hinge region by histone acetyltransferase p300 modulates RORβ stability and transactivation;** Timothy R O'Leary<sup>1</sup>; Ruben D. Garcia-Ordóñez<sup>1</sup>; Patrick R. Griffin<sup>1</sup>; Mi Ra Chang<sup>1</sup>; <sup>1</sup>UF Scripps, Florida, Jupiter, FL
- ThP 714 **Lysine lactylation controls liquid-liquid phase separation and immune signaling during viral infection;** Matthew D Tyl<sup>1</sup>; Victoria Merengwa<sup>1</sup>; Ileana M Cristea<sup>1</sup>; <sup>1</sup>Princeton University, Princeton, NJ

## THURSDAY POSTERS

- ThP 715 **Systematic investigation of the N-terminal effect on protein stability**; Zeyu Wang<sup>1</sup>; Senhan Xu<sup>1</sup>; Kejun Yin<sup>1</sup>; Xing Xu<sup>1</sup>; Ronghu Wu<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA
- PROTEOMICS: CLINICAL APPLICATIONS II**  
**716-737**
- ThP 716 **Mapping phosphorylation of peptide biomarkers corresponding with glioblastoma tumours using data-dependent acquisition and prototype benchtop multi-reflecting time-of-flight mass spectrometry**; Matthew E Daly<sup>1</sup>; Nikki Atwal<sup>1</sup>; Lee A Gethings<sup>1</sup>; Christopher J Hughes<sup>1</sup>; Richard Lock<sup>1</sup>; Nelofer Syed<sup>2</sup>; <sup>1</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>2</sup>Imperial College London, London, United Kingdom
- ThP 717 **The Impact of Maternal Vitamin D Status during Breastfeeding on Human Milk Proteome**; Rony Hull<sup>1</sup>; Jennifer R Bethard<sup>1</sup>; John E Baatz<sup>1</sup>; Katherine Chetta<sup>1</sup>; Danforth A Newton<sup>1</sup>; Carol L Wagner<sup>1</sup>; Lauren E Ball<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC
- ThP 718 **Refining Classification of Cholangiocarcinoma Subtypes via Proteogenomic Integration Reveals New Therapeutic Prospects**; Heeyoun Hwang; Korea Basic Science Institute, cheongju, South Korea
- ThP 719 **Enhanced Detection of Hemoglobin Variants in Clinical Research using Dried Blood Spot and High-Resolution, Accurate-Mass (HRAM) MS**; Yvonne Ehwang Song<sup>1</sup>; Kerry Hassell<sup>1</sup>; Edward Goucher<sup>2</sup>; Jingshu Guo<sup>1</sup>; Tanis Correa<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Hemel Hempstead, United Kingdom
- ThP 720 **An Interlaboratory Comparison of a Highly Multiplexed, Quantitative Peptide Assay to Measure Health Surveillance Panel Proteins in Plasma**; Chi D. L. Nguyen<sup>1</sup>; Matthew Daly<sup>2</sup>; Lee Gethings<sup>2</sup>; Jennifer E. Van Eyk<sup>3</sup>; Susan M. Mockus<sup>4</sup>; <sup>1</sup>Precision Biomarker Laboratories, Cedars Sinai Medical Center, Beverly Hills, CA; <sup>2</sup>Waters Corporation, Wilmslow, United Kingdom; <sup>3</sup>Advanced Clinical BioSystems Research Institute, Cedars-Sinai Medical Center, Los Angeles, California; <sup>4</sup>Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, California
- ThP 721 **High-throughput platelet proteomics from small amounts of previously frozen samples adds another layer to plasma-based immunophenotyping**; Dylan Nicholas T Tabang<sup>1</sup>; Kathrin Korff<sup>1,2</sup>; Kaitlin Brannon<sup>1</sup>; Komal Mandal<sup>1</sup>; Julia Tilburg<sup>3,4</sup>; Patrick Van Zalm<sup>1</sup>; Arthur Viodé<sup>1</sup>; Arjun Ravishanker<sup>5</sup>; Jin Gyu Cheong<sup>6</sup>; Steven Z Josefowicz<sup>5</sup>; Joseph E Italiano<sup>3,4</sup>; Kinga K Smolen<sup>6,7</sup>; Hanno Steen<sup>1,7</sup>; <sup>1</sup>Department of Pathology, Boston Children's Hospital and Harvard Medical School, Boston, MA; <sup>2</sup>Faculty of Chemistry, Aalen University, Aalen, Germany; <sup>3</sup>Department of Surgery, Harvard Medical School, Boston, MA; <sup>4</sup>Vascular Biology Program, Boston Children's Hospital, Boston, MA; <sup>5</sup>Laboratory of Epigenetics and Immunity, Department of Pathology and Laboratory Medicine, Weill Cornell Medicine, New York, NY; <sup>6</sup>Department of Pediatrics, Boston Children's Hospital and Harvard Medical School, Boston, MA; <sup>7</sup>Precision Vaccines Program, Division of Infectious Diseases, Boston Children's Hospital, Boston, MA
- ThP 722 **Multiple reaction monitoring-mass spectrometry-based assay for nondepleted plasma protein quantitation: Application to screening for psychiatric disorders**; Dongyoon Shin<sup>1</sup>; Yeongshin Kim<sup>2</sup>; Junho Park<sup>1,3</sup>; Youngsoo Kim<sup>1,2</sup>; <sup>1</sup>Proteomics Research Team, CHA Institute of Future Medicine, Pangyo, South Korea; <sup>2</sup>Department of Medical Science, School of Medicine, CHA University, Pangyo, South Korea; <sup>3</sup>Department of Pharmacology, School of Medicine, CHA University, Pangyo, South Korea
- ThP 723 **Analysis of HMGB1 protein secreted by lung and colon cancer cells in response to oxaliplatin**; Jingqi Fan<sup>1</sup>; Kevin P. Gillespie<sup>1</sup>; Clementina Mesaros<sup>1</sup>; Ian Alexander Blair<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA
- ThP 724 **High sensitivity measurement of CSF and plasma tau phosphorylation in Alzheimer's disease using Orbitrap Astral mass spectrometer**; Joanna M Kirkpatrick<sup>1</sup>; Laia Montoliu-Gaya<sup>2</sup>; Gunnar Brinkmalm<sup>2</sup>; Eugen Damoc<sup>3</sup>; Tabiwang N Arrey<sup>3</sup>; Bernard Delanghe<sup>3</sup>; Kaj Blennow<sup>2</sup>; Henrik Zetterberg<sup>2</sup>; Johan Gobom<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; <sup>2</sup>Institute of Neuroscience and Physiology, University of Gothenburg, Neurochemistry laboratory SU/Mölndal Hospital, Mölndal, Sweden; <sup>3</sup>Thermo Fisher Scientific, Bremen, Germany
- ThP 725 **Absolute quantification of BRCA1 protein levels in formalin-fixed, paraffin-embedded (FFPE) tissue by FAIMS-PRM**; Beom-Jun Kim<sup>1</sup>; Steve M. Sweet<sup>1</sup>; Camille Lombard-Banek<sup>1</sup>; David C. Chain<sup>1</sup>; Josep V. Forment<sup>2</sup>; Natalia Lukashchuk<sup>2</sup>; Yeoun Jin Kim<sup>1</sup>; <sup>1</sup>AstraZeneca, Gaithersburg, MD; <sup>2</sup>AstraZeneca, Cambridge, United Kingdom
- ThP 726 **Serum Proteome Profiling of Diabetic Patients Treated with Novel Antidiabetics Shows Improved Cognitive Function, Cardiovascular Function, and Reduce Inflammatory Responses**; Md Abdul Hakim<sup>1</sup>; Shams Osman<sup>2</sup>; Akeem Sanni<sup>1</sup>; Waziha Purba<sup>1</sup>; Md Mostofa Al Amin Bhuiyan<sup>1</sup>; Sherifdeen Onigbinde<sup>1</sup>; Arvin Saffarian Delkosh<sup>1</sup>; Ahmed El-Yazbi<sup>3</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; <sup>2</sup>Department of Clinical Pharmacy and Pharmacy Practice, Faculty of Pharmacy, Alexandria University, Alexandria, Egypt; <sup>3</sup>Department of Pharmacology and Therapeutics, Faculty of Pharmacy, Alamein International University, Alamein, Egypt
- ThP 727 **Exploring the Impact of Fasting on Biological Pathways through LC-MS/MS of Profiling Serum Proteome**; Md Mostofa Al Amin Bhuiyan<sup>1</sup>; Waziha Purba<sup>1</sup>; Md Abdul Hakim<sup>1</sup>; Ayobami Oluokun<sup>1</sup>; Ahmed Elyazbi<sup>2</sup>; Haneen S. Dwaib<sup>3</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; <sup>2</sup>Department of Pharmacology and Therapeutics, Faculty of Pharmacy, Alamein International University, Alamein, Egypt; <sup>3</sup>Clinical Nutrition Department, Palestine Ahliya University, Bethlehem, Palestine
- ThP 728 **Conventional anticoagulants allow preanalytical variation that confounds the accuracy of plasma proteomics**; Rachel M Miller<sup>1</sup>; Sama Mehta<sup>1</sup>; Xiaoyuan Zhou<sup>2</sup>; Nicholas Mucci<sup>2</sup>; Ryan W. Benz<sup>2</sup>; Jing Li<sup>1</sup>; <sup>1</sup>Streck LLC., La Vista, NE; <sup>2</sup>Seer Inc., Redwood City, CA
- ThP 729 **Fucoidan ameliorates skin fibrosis via tight junction regulation**; Pang-Hung Hsu; National Taiwan Ocean University, Keelung, Taiwan
- ThP 730 **Proteome and Tau Profiles in Extracellular Vesicles Derived from Brain Fluid among human tauopathies by mass spectrometry**; Laura Fichter<sup>1</sup>; Elodie Leroux<sup>2</sup>; Marie Oosterlynck<sup>2</sup>; Morvane Colin<sup>2</sup>; Jérôme Vialaret<sup>3</sup>; Sylvain Lehmann<sup>3</sup>; Luc Buée<sup>2</sup>; Christophe Hirtz<sup>3</sup>; <sup>1</sup>PPC - CHU de Montpellier, Montpellier, France; <sup>2</sup>Alzheimer et Tauopathies, Lille Neuroscience & Cognition, Lille, France; <sup>3</sup>PPC - CHU de Montpellier, MONTPELLIER, France
- ThP 731 **Identification of blood group variants using RBC ghost membrane proteomics**; Ankit P Jain<sup>1</sup>; Anne Roberts<sup>1</sup>; Lilian R Heil<sup>2</sup>; John D Roback<sup>1,3</sup>; Blaine Roberts<sup>1</sup>; <sup>1</sup>Emory University School of Medicine, Atlanta, GA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Emory University Hospital, Atlanta, GA
- ThP 732 **Efficient Human Plasma Proteome Profiling at up to 300 Samples Per Day**; Paul Jacobs<sup>1</sup>; Jeff Op De Beeck<sup>2</sup>; Robert Van Ling<sup>3</sup>; Yuan Lin<sup>4</sup>; Shanhua Lin<sup>4</sup>; <sup>1</sup>Thermo Fisher Scientific - Belgium, Ghent, Belgium; <sup>2</sup>Thermo Fisher Scientific, Ghent, Belgium; <sup>3</sup>Thermo Fisher Scientific - Breda, Breda, Netherlands; <sup>4</sup>Thermo Fisher Scientific, Sunnyvale, CA
- ThP 733 **Fast-tracking the journey to targeted clinical assays with a novel hybrid high-speed nominal mass instrument**; Maria Wahle<sup>1</sup>; Vincent Albrecht<sup>1</sup>; Johannes Mueller-Reif<sup>1</sup>; Philip M. Remes<sup>2</sup>; Cristina Jacob<sup>2</sup>; Claudia Martins<sup>2</sup>; Stevan

## THURSDAY POSTERS

- Horning<sup>3</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>Department of Proteomics and signal Transduction, Max-Planck-Institute of Biochemistry, Martinsried (near Munich), Germany; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- ThP 734 **Merits of bacterial classification with microflow LC-MS/MS;** Miriam Abele<sup>1, 2</sup>; Armin Soleymaniniya<sup>3</sup>; Etienne Doll<sup>4</sup>; Siegfried Scherer<sup>4</sup>; Klaus Neuhaus<sup>5</sup>; Nina Wantia<sup>6</sup>; Mathias Wilhelm<sup>3</sup>; Bernhard Kuster<sup>1, 2</sup>; Christina Ludwig<sup>1</sup>; <sup>1</sup>Bavarian Center for Biomolecular Mass Spectrometry, TU Munich, TUM School of Life Sciences, Freising, Germany; <sup>2</sup>Chair of Proteomics and Bioanalytics, TU Munich, TUM School of Life Sciences, Freising, Germany; <sup>3</sup>Computational Mass Spectrometry, TU Munich, TUM School of Life Sciences, Freising, Germany; <sup>4</sup>Chair of Microbial Ecology, TU Munich, TUM School of Life Sciences, Freising, Germany; <sup>5</sup>Core Facility Microbiome, ZIEL Institute for Food & Health, TU Munich, Freising, Germany; <sup>6</sup>Institut für Medizinische Mikrobiologie, Immunologie und Hygiene, TUM School of Medicine and Health, TU Munich, München, Germany
- ThP 735 **Deep plasma protein profiling enabled by nanoparticle-based sample preparation and Orbitrap Astral mass spectrometer;** William F Beimers<sup>1</sup>; Katherine A Overmyer<sup>1, 2, 3</sup>; Rachael Wilson<sup>4, 5</sup>; Sterling C Johnson<sup>4, 5, 6</sup>; Joshua J Coon<sup>1, 2, 3, 7</sup>; <sup>1</sup>Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Morgridge Institute for Research, Madison, WI; <sup>3</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI; <sup>4</sup>Wisconsin Alzheimer's Institute, Madison, WI; <sup>5</sup>Wisconsin Alzheimer's Disease Research Center, Madison, WI; <sup>6</sup>Department of Medicine, University of Wisconsin-Madison, Madison, WI; <sup>7</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- ThP 736 **Quantification of the PD-1/PD-L1 Axis in Various Cancer Types by Immuno-Multiple Reaction Monitoring;** Neda Boushehri<sup>1, 2</sup>; Vincent Lacasse<sup>1, 3</sup>; Alan Spatz<sup>3, 4</sup>; Robert Popp<sup>5</sup>; Rene P. Zahedi<sup>6, 7, 8, 9</sup>; Kevin Kunhong Xiao<sup>10</sup>; Patrick L. Wagner<sup>10</sup>; Sitara Niranjan<sup>10</sup>; Rachel Dileo<sup>10</sup>; Huseyin Sakib Karakilic<sup>10</sup>; Amanjit Gil<sup>10</sup>; Christoph H. Borchers<sup>1, 2, 3, 4</sup>; <sup>1</sup>Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; <sup>2</sup>Division of Experimental Medicine, McGill University, Montreal, QC; <sup>3</sup>Department of Pathology, McGill University, Montreal, QC; <sup>4</sup>Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; <sup>5</sup>MRM Proteomics Inc, Montreal, QC; <sup>6</sup>Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; <sup>7</sup>Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; <sup>8</sup>Department of Internal Medicine, University of Manitoba, Winnipeg, MB; <sup>9</sup>CancerCare Manitoba Research Institute, Winnipeg, MB; <sup>10</sup>Allegheny Health Network Cancer Institute, Pittsburgh, PA
- ThP 737 **A large-scale DIA-MS acquisition of iPSC-derived motor neurons;** Oliver Y Wang<sup>1</sup>; Oleg A. Karpov<sup>1</sup>; Niveda Sundaraman<sup>1</sup>; Rakhi Pandey<sup>1</sup>; Velina Kozareva<sup>2</sup>; Stanislav Tsitkov<sup>2</sup>; Dhruv Sareen<sup>1</sup>; Ernest Fraenkel<sup>2</sup>; Clive Svendsen<sup>1</sup>; Jennifer E. Van Eyk<sup>1</sup>; <sup>1</sup>Cedars-Sinai Medical Center, Los Angeles, CA; <sup>2</sup>Massachusetts Institute of Technology, Cambridge, MA
- PROTEOMICS: INTACT PROTEINS AND TOP DOWN ANALYSIS II**  
738-767
- ThP 738 **Combinatorial Probabilities of Multiple Fragmentations Explain Polypeptide MS/MS Intensity Distribution, Overrepresentation of Smaller Fragments, and Missing Middle of Top-Down MS;** Wensheng Yang<sup>1</sup>; Novera Alam<sup>1</sup>; Jeffrey Agar<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA
- ThP 739 **Optimization of TDMS analysis of proteoforms from membrane-bound particles for future translational studies based on human plasma;** Amal Mohamed Kamal Eltobshi<sup>1</sup>; Jake Kline<sup>1</sup>; Luca Fornelli<sup>1</sup>; <sup>1</sup>University of Oklahoma, Norman, OK
- ThP 740 **Fast and Robust Proteoforms Platform Development via Immunoaffinity Purifications Coupling to Top-Down Mass Spectrometry (IP-MS) for Biomarkers Precision Medicine;** Nadia Sultana<sup>1</sup>; Baoliang Cui<sup>1</sup>; Khader Awwad<sup>1</sup>; Michael Schulz<sup>1</sup>; Qin Ji<sup>1</sup>; Mario Richter<sup>1</sup>; Yu Tian<sup>1</sup>; <sup>1</sup>Research & Development, AbbVie, North Chicago, IL
- ThP 741 **Evaluation of Intact Protein Extraction Strategies in Top-Down Proteomics;** Xingzhao Xiong<sup>1</sup>; Xiaowen Liu<sup>1</sup>; <sup>1</sup>Tulane University, New Orleans, LA
- ThP 742 **Deep Profiling of Plasma Proteoforms with Engineered Nanoparticles for Top-down Proteomics Analysis;** Che-Fan Huang<sup>1</sup>; Aniel Sanchez<sup>1</sup>; Mrittika Bhattacharya<sup>2</sup>; Giang Ho<sup>2</sup>; Ambika Sundaresan<sup>2</sup>; Michael A. Hollas<sup>1</sup>; Michael A. Caldwell<sup>1</sup>; Xiaoyan Zhao<sup>2</sup>; Ryan W. Benz<sup>2</sup>; Asim Siddiqui<sup>2</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Seer Inc., Redwood City, CA
- ThP 743 **Demultiplexing of Top-down Data-Dependent Acquisition Mass Spectrometry;** Zhige Wang<sup>1</sup>; Xingzhao Xiong<sup>1</sup>; Xiaowen Liu<sup>1</sup>; <sup>1</sup>Tulane University, New Orleans, LA
- ThP 744 **Developing Advanced Capillary Zone Electrophoresis-Mass Spectrometry Techniques for Multi-Level Proteomics of Complex Biological Samples;** Qianyi Wang<sup>1</sup>; Qianjie Wang<sup>1</sup>; Zihao Qi<sup>2</sup>; William Moeller<sup>2</sup>; Shaolei Lu<sup>3</sup>; Xiaowen Liu<sup>4</sup>; Chiung-Kuei Huang<sup>4</sup>; Vicki Wysocki<sup>2</sup>; Liangliang Sun<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI; <sup>2</sup>Ohio State University, Columbus, OH; <sup>3</sup>Brown University, Providence, RI; <sup>4</sup>Tulane University, New Orleans, LA
- ThP 745 **Single-shot native top-down proteomics on the Corynebacterium diphtheriae exoproteome reveals novel proteoforms, complexes, and functional heme-acquisition system components;** Andrew K Goring<sup>1</sup>; Jordan Ford<sup>1</sup>; Christopher Mullen<sup>2</sup>; Jingjing Huang<sup>2</sup>; Rafael Melani<sup>2</sup>; Robert T. Clubb<sup>1</sup>; Rachel R. Ogorzalek Loo<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>University of California, Los Angeles, Los Angeles, CA; <sup>2</sup>ThermoFisher Scientific, San Jose, CA
- ThP 746 **Protein-centric analysis of personalized antibody repertoires – LC-MS-based Fab-profiling on a timsTOF;** Jan Fiala<sup>1, 2</sup>; Dina Schuster<sup>1, 2</sup>; Simon Ollivier<sup>1, 2</sup>; Stuart Pengelley<sup>3</sup>; Markus Lubeck<sup>3</sup>; Florian Busch<sup>4</sup>; Oliver Raether<sup>3</sup>; Jean-François Greisch<sup>4</sup>; Albert J.R. Heck<sup>1, 2</sup>; <sup>1</sup>Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht University, Padualaan 8, 3584 CH, Utrecht, Netherlands; <sup>2</sup>Netherlands Proteomics Center, Padualaan 8, 3584 CH Utrecht, Netherlands; <sup>3</sup>Bruker Daltonik GmbH & Co. KG, Bremen, Germany; <sup>4</sup>Bruker Daltonik GmbH, Fällanden, Switzerland
- ThP 747 **MASS SPECTROMETRY OF PROTEINS AND PROTEIN COMPLEXES ELECTROSPRAYED FROM PHYSIOLOGICALLY RELEVANT CONDITIONS AIDED BY GAS-PHASE METHODS;** Erick G Baez Bolivar; Purdue University, West Lafayette, IN
- ThP 748 **An Optimized High-Throughput Top-Down Proteomic Method to Characterize Recombinant RAS Modifications;** Grace M. Scheidemantle<sup>1</sup>; Robert A. D'Ippolito<sup>1</sup>; Matthew R. Drew<sup>1</sup>; Peter Frank<sup>1</sup>; Min Hong<sup>1</sup>; Jennifer Mehalko<sup>1</sup>; Simon Messing<sup>1</sup>; Shelley Perkins<sup>1</sup>; Kelly Snead<sup>1</sup>; Vanessa Wall<sup>1</sup>; Carissa Grose<sup>1</sup>; William Burgan<sup>1</sup>; Dominic Esposito<sup>1</sup>; Frank McCormick<sup>1, 2</sup>; Dwight V. Nissley<sup>1</sup>; Caroline J. DeHart<sup>1</sup>; <sup>1</sup>Frederick National Laboratory, Frederick, MD; <sup>2</sup>Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA
- ThP 749 **Analysis of intact membrane proteins directly from living bacterial colonies by native LESA mass spectrometry;** Yuying Du<sup>1</sup>; Robin May<sup>1</sup>; Helen Cooper<sup>1</sup>; <sup>1</sup>University of Birmingham, Birmingham, United Kingdom
- ThP 750 **High Sensitivity Top-down Proteomics for Analysis of Large Proteoforms Enabled by Small-scale Serial Size Exclusion Chromatography;** Holden T Rogers<sup>1</sup>; Jake A Melby<sup>1</sup>; Lauren E Ehlers<sup>1</sup>; Matthew S Fischer<sup>1</sup>; Eli J Larson<sup>1</sup>; Zhan Gao<sup>2</sup>; Kalina J Rossler<sup>2</sup>; Daojing Wang<sup>3</sup>; Andrew J Alpert<sup>4</sup>; Ying Ge<sup>2, 5</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin; <sup>2</sup>University of Wisconsin-Madison, Department of Cell and Regenerative



## THURSDAY POSTERS

- Biology, Madison, WI; <sup>3</sup>Newomics Inc., Berkeley, CA; <sup>4</sup>PolyLC Inc, Columbia, MD; <sup>5</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, WI
- ThP 751 **Exploration of Structural and Relative Stability Information of Protein Complexes by Utilizing D-proline and Native Top-Down MS;** Luchen Wuyang<sup>1</sup>; Boyu Zhao<sup>1</sup>; Rachel Loo<sup>1</sup>; Joseph Loo<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles, California
- ThP 752 **Site-Selective Cleavage of Proteins by Radical Photoactivation;** Chengwei Chen<sup>1</sup>; Ryan R. Julian<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA
- ThP 753 **A simple and efficient approach for preparing cationic capillary coating for capillary electrophoresis-mass spectrometry-based top-down proteomics;** Qianjie Wang<sup>1, 2</sup>; Guangyao Gao<sup>1</sup>; Peter Lundquist<sup>2</sup>; Liangliang Sun<sup>1</sup>; <sup>1</sup>Department of Chemistry, Michigan State University, East Lansing, MI; <sup>2</sup>Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI
- ThP 754 **Identification and Verification of Plasma Proteoform Markers from Patients with Progressive Liver Cirrhosis;** Aniel Sanchez<sup>1</sup>; Eleonora Forte<sup>1, 2</sup>; Indira Pla<sup>1</sup>; Che-Fan Huang<sup>1</sup>; Vijaya Lakshmi Kanchustambham<sup>1</sup>; Michael A. Hollas<sup>1</sup>; Troy D Fisher<sup>1</sup>; Katrina N Peterson<sup>1</sup>; Jes M Sanders<sup>2</sup>; Julianna M Doll<sup>2</sup>; Zachary C Dietch<sup>2</sup>; Rafael D Melani<sup>3</sup>; Daniela P Ladner<sup>2</sup>; Michael W Senko<sup>3</sup>; Neil L Kelleher<sup>1, 2</sup>; <sup>1</sup>Proteomics Center of Excellence, Northwestern University, Evanston, Illinois; <sup>2</sup>Comprehensive Transplant Center, Feinberg School of Medicine, Northwestern University, Chicago, Illinois; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 755 **Evaluating a new Workflow for Top-Down Protein Sequence Confirmation and de novo Sequencing;** Mariangela Kosmopoulou<sup>1</sup>; George Alevizos<sup>1</sup>; Georgia Orfanoudaki<sup>1</sup>; Athanasios Smyrnakis<sup>1</sup>; Michael Greig<sup>2</sup>; Detlev Suckau<sup>3</sup>; <sup>1</sup>Fasmatech Science and Technology, Athens, Greece; <sup>2</sup>Bruker Scientific, 40 Manning Road, Billerica, MA; <sup>3</sup>Bruker Daltonics, Bremen, Germany
- ThP 756 **Advancing FDR Estimation for Spectral Deconvolution in Top-Down Proteomics;** Avesha Feroz<sup>1</sup>; Timo Sachsenberg<sup>1, 2</sup>; Konstantin O. Nagornov<sup>3</sup>; Yury O. Tsybin<sup>3</sup>; Oliver Kohlbacher<sup>1, 2, 4</sup>; Kyowon Jeong<sup>1, 2</sup>; <sup>1</sup>Applied Bioinformatics, Department for Computer Science, University of Tübingen, Sand 14, 72076, Tübingen, Germany; <sup>2</sup>Institute for Bioinformatics and Medical Informatics, University of Tübingen, Sand 14, 72076, Tübingen, Germany; <sup>3</sup>Spectroswiss, 1015, Lausanne, Switzerland; <sup>4</sup>Translational Bioinformatics, University Hospital Tübingen, Hoppe-Seyler-Str. 9, 72076, Tübingen, Germany
- ThP 757 **Novel capillary isoelectric focusing-mass spectrometry techniques for top-down proteomics characterization of histones and nanoparticle protein corona;** Guijie Zhu<sup>1</sup>; Fei Fang<sup>1</sup>; Amirhossein Sadeghi<sup>1</sup>; Liangliang Sun<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI
- ThP 758 **FLASHTagger: An open-source web application utilizing de novo sequence tags for robust and ion type-free analysis of top-down data;** Kyowon Jeong<sup>1, 2</sup>; Wonhyeuk Jung<sup>3, 4</sup>; Jaywon Lee<sup>3, 4</sup>; Aniruddha Panda<sup>3, 4</sup>; Jared Shaw<sup>5</sup>; Tom D. Müller<sup>1, 2</sup>; Louise M Buur<sup>6</sup>; Viktoria Dorfer<sup>6</sup>; Oliver Kohlbacher<sup>1, 2, 7</sup>; Kallol Gupta<sup>3, 4</sup>; <sup>1</sup>Applied Bioinformatics, Department for Computer Science, University of Tübingen, Sand 14, 72076, Tübingen, Germany; <sup>2</sup>Institute for Bioinformatics and Medical Informatics, University of Tübingen, Sand 14, 72076, Tübingen, Germany; <sup>3</sup>Yale School of Medicine, New Haven, CT; <sup>4</sup>Nanobiology Institute, Yale University, West Haven, CT; <sup>5</sup>University of Nebraska - Lincoln, Lincoln, NE; <sup>6</sup>University of Applied Sciences Upper Austria, Hagenberg, Austria; <sup>7</sup>Translational Bioinformatics, University Hospital Tübingen, Hoppe-Seyler-Str. 9, 72076, Tübingen, Germany
- ThP 759 **Quantification of age-related proteoform expression changes in cardiac mitochondria using quantitative top-down proteomics;** Kellye A Cupp-Sutton<sup>1</sup>; Anju Teresa Sunny<sup>1</sup>; Andrea Ramirez-Sagredo<sup>2</sup>; Ann Chiao<sup>2</sup>; Si Wu<sup>1, 3</sup>; <sup>1</sup>University of Alabama, Tuscaloosa, AL; <sup>2</sup>Oklahoma Medical Research Foundation, Oklahoma City, Oklahoma; <sup>3</sup>University of Oklahoma, Norman, OK
- ThP 760 **High-precision Proteoform Quantification Reveals Phosphorylation Kinetics of AMP-activated Protein Kinase;** Boris Krichel<sup>1, 2</sup>; Hsin-Ju Chan<sup>1</sup>; Zhan Gao<sup>1</sup>; Charlotte Uetrecht<sup>2, 3</sup>; Ying Ge<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI; <sup>2</sup>University of Siegen, Siegen, Germany; <sup>3</sup>Centre for Structural Systems Biology, Hamburg, Germany
- ThP 761 **Effect of Charge-State Manipulation on Protein Conformation;** Dmitry Eremin<sup>1</sup>; Brandon Nelson<sup>2</sup>; Joshua K McBee<sup>2</sup>; Ashli R Simone<sup>2</sup>; Daniel DeBord<sup>2</sup>; Valery Fokin<sup>1</sup>; <sup>1</sup>University of Southern California, Los Angeles, CA; <sup>2</sup>MOBILion Systems, Inc., Chadds Ford, PA
- ThP 762 **Enhancing top-down proteomics by novel separation columns coupled to mass spectrometry;** Yu Liang<sup>1</sup>; Yue Sun<sup>1</sup>; Chao Wang<sup>1</sup>; Zhen Liang<sup>1</sup>; Lihua Zhang<sup>1</sup>; Yukui Zhang<sup>1</sup>; <sup>1</sup>Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China
- ThP 763 **Validating Matching Terminal and Internal Fragments from Targeted Top-Down Proteoform Analyses;** Joseph B. Greer<sup>1, 2</sup>; Bryan P. Early<sup>1, 2</sup>; Daisha Utley<sup>1</sup>; Jessie A. Bolger<sup>1</sup>; Matthew T. Robey<sup>1, 2</sup>; Ryan T. Fellers<sup>1, 2</sup>; Neil L. Kelleher<sup>2</sup>; Kenneth R. Durbin<sup>1, 2</sup>; <sup>1</sup>Proteinacious, Evanston, IL; <sup>2</sup>Northwestern University, Evanston, IL
- ThP 764 **Characterizing Intact Antibodies Using Ultrafast Sliding Window Deconvolution;** Matthew T. Robey<sup>1</sup>; Daisha Utley<sup>1</sup>; Joseph B. Greer<sup>1, 2</sup>; Ryan T. Fellers<sup>1, 2</sup>; Neil L. Kelleher<sup>1, 2</sup>; Kenneth R. Durbin<sup>1, 2</sup>; <sup>1</sup>Proteinacious, Evanston, IL; <sup>2</sup>Northwestern University, Evanston, IL
- ThP 765 **Dissecting protein-protein interactions and defining the composition of novel proteoforms in a G protein-coupled receptor signalling cascade using native top-down;** Corinne Lutomski<sup>1</sup>; Jack L Bennett<sup>1</sup>; Tarick J El-Baba<sup>1</sup>; Di Wu<sup>1</sup>; Joshua D. Hinkle<sup>2</sup>; Christopher Mullen<sup>2</sup>; John E.P. Syka<sup>2</sup>; Idlir Liko<sup>3</sup>; Carol V Robinson<sup>1</sup>; <sup>1</sup>University of Oxford, Oxford, United Kingdom; <sup>2</sup>ThermoFisher Scientific, San Jose, CA; <sup>3</sup>OMass Therapeutics, Oxford, United Kingdom
- ThP 766 **EXPLORING THE MECHANISM OF MIDDLE DOWN ELECTRON ACTIVATED DISSOCIATION BASED SEQUENCING OF MULTISPECIFIC ANTIBODIES;** Michael L. Poltash<sup>1</sup>; Haichuan Liu<sup>2</sup>; Zoe Zhang<sup>2</sup>; Andrew D Mahan<sup>1</sup>; Hirsh Nanda<sup>1</sup>; <sup>1</sup>Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania; <sup>2</sup>SCIEX, Redwood City, CA
- ThP 767 **MALDI mass analysis of 26S proteasome and its subunits using MALDI linear ion trap mass spectrometry;** Avinash Adhikrao Patil<sup>1</sup>; Ching-Chieh Lee<sup>2</sup>; Wen-Ping Peng<sup>2</sup>; <sup>1</sup>National Dong Hwa University, Shoufeng, Taiwan; <sup>2</sup>National Dong Hwa University, Shoufeng, Hualien, Taiwan

### PROTEOMICS: QUANTITATIVE II 768-799

- ThP 768 **Quantification of complement membrane attack complex proteins in plasma extracellular vesicles;** Illarion Turko; <sup>1</sup>Institute for Bioscience and Biotechnology Research, Rockville, MD
- ThP 769 **Real-time peptide-spectrum rescoring improves sensitivity for sample multiplexed proteomics;** Chris McGann<sup>1</sup>; Erik Bergstrom<sup>1</sup>; Devin Schweppe<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA
- ThP 770 **Establishing a low-input mouse immune cell proteomic atlas with unit-resolution mass spectrometry for targeted library generation;** Ariana E Shannon<sup>1</sup>; Nojoon Soon<sup>1</sup>; Yi Wang<sup>1</sup>; Teeradon Phlairaharn<sup>2</sup>; Lilian R Heil<sup>3</sup>; Cristina Jacob<sup>3</sup>; Philip M. Remes<sup>3</sup>; Brian Searle<sup>1</sup>; <sup>1</sup>The Ohio State University, Columbus, OH; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 771 **Quantifying the metabolic proteome;** Yassene Mohammed<sup>1, 2, 3</sup>; Vincent R. Richard<sup>1</sup>; Claudia Gaither<sup>4</sup>; Robert Popp<sup>4</sup>; Christoph H. Borchers<sup>1, 3, 5, 6</sup>; <sup>1</sup>Segal Cancer

## THURSDAY POSTERS

- Proteomics Centre, Jewish General Hospital, Montreal, QC;*  
<sup>2</sup>*Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands;*  
<sup>3</sup>*Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC;*  
<sup>4</sup>*MRM Proteomics Inc, Montreal, QC;*  
<sup>5</sup>*Division of Experimental Medicine, McGill University, Montreal, QC;*  
<sup>6</sup>*Department of Pathology, McGill University, Montreal, QC*
- ThP 772 **Deep, unbiased and quantitative mass spectrometry-based plasma proteome analyses of personalized response to mRNA COVID-19 vaccine;** Ting Huang<sup>1</sup>; Alex Rosa Campos<sup>2</sup>; Jian Wang<sup>1</sup>; Alexey Stukalov<sup>1</sup>; Ramón Díaz<sup>3</sup>; Svetlana Maurya<sup>3</sup>; Khatereh Motamedchaboki<sup>1</sup>; Daniel Hornburg<sup>1</sup>; Laura R. S. Oliveira<sup>4</sup>; Camila I. Alves<sup>4</sup>; Rafael L. Rosa<sup>4</sup>; Yohana P. Calegari-Alves<sup>4</sup>; Serafim Batzoglou<sup>1</sup>; Lucélia Santi<sup>4</sup>; Walter O. Beys-da-Silva<sup>4</sup>; <sup>1</sup>*Seer, Inc., Redwood City, CA;* <sup>2</sup>*Plexium, San Diego, CA;* <sup>3</sup>*Sanford Burnham Prebys, San Diego, California;* <sup>4</sup>*Federal University of Rio Grande do Sul, Porto Alegre, Brazil*
- ThP 773 **Providing an analytical platform for state-of-the-art absolute apolipoprotein quantification in human blood plasma using prm-PASEF;** David Kotol<sup>1</sup>; Christian Albers<sup>2</sup>; Stephanie Kaspar-Schoenfeld<sup>2</sup>; <sup>1</sup>*ProteomEdge, Stockholm, Sweden;* <sup>2</sup>*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*
- ThP 774 **Exploring Human Serum Proteome Profiles in Response to Chronic and Acute Exposure to Organophosphate Pesticides using LC-MS/MS;** Moigan Atashi<sup>1</sup>; Dina El-Gameel<sup>2</sup>; Vishal Sandilya<sup>1</sup>; Thu Nguyen<sup>1</sup>; Md Mostofa Al Amin Bhuiyan<sup>1</sup>; Judith Ijeoma Nwaiwu<sup>1</sup>; Noha A. Hamdy<sup>3</sup>; Maha A. Ghanem<sup>4</sup>; Labiba K El-Khordaugi<sup>3</sup>; Salwa M. Abdallah<sup>5</sup>; Ahmed El-Yazbi<sup>6</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>*Texas Tech University, Lubbock, Texas;* <sup>2</sup>*Alexandria University Hospitals, Alexandria, Egypt;* <sup>3</sup>*Faculty of Pharmacy, Alexandria University, Alexandria, Egypt;* <sup>4</sup>*Faculty of Medicine, Alexandria University, Alexandria, Egypt;* <sup>5</sup>*Central Agricultural Pesticides Lab (CAPL), Agricultural Research Center (ARC), Cairo, Egypt, Cairo, Egypt;* <sup>6</sup>*Department of Pharmacology and Therapeutics, Faculty of Pharmacy, Alamein International University, Alamein, Egypt*
- ThP 775 **Amyotrophic Lateral Sclerosis-Associated Mutants of SOD1 Altered mRNA Splicing through Their Aberrant Interactions with SRSF2;** Xingyuan Chen<sup>1</sup>; Zhongwen Cao<sup>1</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>*University of California, Riverside, Riverside, CA*
- ThP 776 **Real-Time Search enables sensitive and accurate TMTproC quantification of transcription factors during embryogenesis;** Alex Johnson<sup>1</sup>; Jingjing Huang<sup>2</sup>; Argit Marishta<sup>1</sup>; Edward Cruz<sup>1</sup>; Andrea Mariosi<sup>1</sup>; William Barshop<sup>2</sup>; Jesse D. Canterbury<sup>2</sup>; Rafael Melani<sup>2</sup>; David Bergen<sup>2</sup>; Vlad Zabrovskov<sup>2</sup>; Graeme McAlister<sup>2</sup>; Martin Wühr<sup>1</sup>; <sup>1</sup>*Princeton University, Princeton, NJ;* <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- ThP 777 **Multi-modal proteome atlas to enhance treatment capability of KRAS-driven cancers;** Syed Azmal Ali<sup>1</sup>; Karim Aljakouch<sup>1</sup>; Jeroen Krijgsveld<sup>1, 2</sup>; <sup>1</sup>*German Cancer Research Center, Heidelberg, Germany;* <sup>2</sup>*Heidelberg University, Medical Faculty, Heidelberg, Germany*
- ThP 778 **Characterization of aging-related adaptive naïve and innate immune human proteomes;** Ceereena Ubaida-Mohien<sup>1</sup>; Alexey Lyashkov<sup>1</sup>; Amit Singh<sup>1</sup>; Mary Kaileh<sup>1</sup>; Arsun Bektas<sup>1</sup>; Yevgeniya Lukyanenko<sup>1</sup>; Jaekwan Kim<sup>1</sup>; Julián Candia<sup>1</sup>; Nan Ping Weng<sup>1</sup>; Ranjan Sen<sup>1</sup>; Luigi Ferrucci<sup>1</sup>; <sup>1</sup>*National Institute on Aging, National Institutes of Health, Baltimore, MD 21224*
- ThP 779 **Metabolic labeling to describe extracellular matrix proteome dynamics in a fibrin-based in vitro wound healing model;** Dalton Miles<sup>1</sup>; Kathryn Jacobson<sup>2</sup>; Adrian Buganza-Tepole<sup>3</sup>; Sarah Calve<sup>1</sup>; <sup>1</sup>*University of Colorado Boulder, Boulder, CO;* <sup>2</sup>*University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA;* <sup>3</sup>*Purdue University, West Lafayette, IN*
- ThP 780 **Optimization of narrow isolation windows with Zeno SWATH-DIA for improving proteomic identification;** Kongxin Gu<sup>1</sup>; Haruka Kumabe<sup>1</sup>; Takumi Yamamoto<sup>1</sup>; Naoto Tashiro<sup>1</sup>; Takashi Masuda<sup>2</sup>; Shingo Ito<sup>1</sup>; Sumio Ohtsuki<sup>1</sup>; <sup>1</sup>*Kumamoto University, Kumamoto, Japan;* <sup>2</sup>*Keio University, Tsuruoka, Japan*
- ThP 781 **Targeted proteomics reveals the regulation of the Polycomb Repressive Complex 1 by USP7 and its involvement in neurodevelopment;** Joyce Wolf Van Der Meer<sup>1</sup>; Ayestha Sijm<sup>1</sup>; Axelle Larue<sup>2</sup>; Yaser Atlasi<sup>2</sup>; Jan A Van Der Knaap<sup>1</sup>; Gillan E Chalkley<sup>1</sup>; Karel Bezstarosti<sup>1</sup>; Dick HW Dekkers<sup>1</sup>; Wouter AS Doff<sup>1</sup>; Zeliha Ozgur<sup>1</sup>; Wilfred FJ Van Ijcken<sup>1</sup>; Peter C Verrijzer<sup>1</sup>; Jeroen AA Demmers<sup>1</sup>; <sup>1</sup>*Erasmus University Medical Center, Rotterdam, Netherlands;* <sup>2</sup>*Queen's University Belfast, Belfast, United Kingdom*
- ThP 782 **Global proteomics and integrative thermal proteome profiling of hepatic stellate cells in liver fibrogenesis;** Lan Green<sup>1</sup>; James Rooney<sup>1</sup>; Chunna Guo<sup>1</sup>; Whitney Smith-Kinnaman<sup>1</sup>; Jessica Maiers<sup>1</sup>; Amber L Mosley<sup>1</sup>; <sup>1</sup>*Indiana University School of Medicine, Indianapolis, IN*
- ThP 783 **Accurate multiplexed proteomics on a quadrupole-ion trap instrument;** Edward R Cruz<sup>1</sup>; Alex Johnson<sup>1</sup>; Thao Nguyen<sup>1</sup>; Jessica Wang<sup>1</sup>; Michael Stadlmeier<sup>1</sup>; Philip M Remes<sup>2</sup>; Graeme McAlister<sup>2</sup>; Martin Wühr<sup>1</sup>; <sup>1</sup>*Princeton University, Princeton, NJ;* <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- ThP 784 **Bayesian Confidence Intervals for Absolute Protein Quantification;** Vyas Pujari<sup>1, 2</sup>; Chirag Kumar<sup>1, 2</sup>; Meera Gupta<sup>1, 2</sup>; Donovan Cassidy-Nolan<sup>1, 2</sup>; Arjuna Subramanian<sup>1, 2</sup>; Martin Wühr<sup>1, 2</sup>; <sup>1</sup>*Princeton University, Princeton, NJ;* <sup>2</sup>*Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ*
- ThP 785 **The Association of Biomolecular Resource Facilities Proteomics Standards Research Group (sPRG) Multi-Species Standard to Assist Quantitative Proteomics;** Benjamin A. Neely<sup>1</sup>; Josue Baeza<sup>2</sup>; Magnus Palmblad<sup>3</sup>; Lindsay K Pino<sup>4</sup>; Brian C Searle<sup>5</sup>; Susan T. Weintraub<sup>6</sup>; <sup>1</sup>*National Institute of Standards and Technology, Charleston, SC;* <sup>2</sup>*GSK, Collegeville, PA;* <sup>3</sup>*Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands;* <sup>4</sup>*Talus Bioscience, Seattle, WA;* <sup>5</sup>*Department of Biomedical Informatics, The Ohio State University Medical Center, Columbus, OH;* <sup>6</sup>*Univ. of Texas HSC, San Antonio, TX*
- ThP 786 **A cross-species Proteomic assessment of cost-effective platforms for depleting high-abundant proteins from blood serum;** Zongkai Peng<sup>1</sup>; Shakya Sankalpani Gunasena Wijesunilake<sup>1</sup>; Deepti Bhusal<sup>1</sup>; Isabella Yang<sup>2</sup>; Zhibo Yang<sup>1</sup>; Nagib Ahsan<sup>1, 3</sup>; <sup>1</sup>*Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK;* <sup>2</sup>*Norman North Highschool, Norman, OK;* <sup>3</sup>*Mass Spectrometry, Proteomics and Metabolomics Core Facility, Stephenson Life Sciences Research Center, The University of Oklahoma, Norman, OK*
- ThP 787 **Democratizing Plasma Proteomics: Massively Parallel Targeted Analysis Using a Novel Hybrid Nominal Mass Resolution Tandem Mass Spectrometer;** Christine C. Wu<sup>1</sup>; Philip M. Remes<sup>2</sup>; Cristina C. Jacob<sup>2</sup>; Deanna Plubell<sup>1</sup>; Lillian R Heil<sup>2</sup>; Bo Wen<sup>1</sup>; Nicholas Shulman<sup>1</sup>; Brendan MacLean<sup>1</sup>; Michael MacCoss<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA;* <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- ThP 788 **Translation of Proteograph XT Nanoparticle-Enriched Plasma proteomic features to a targeted assay;** Yi (Jimmy) Zeng<sup>1</sup>; Philip M Remes<sup>2</sup>; Cristina C. Jacob<sup>2</sup>; Hao Qian<sup>1</sup>; Megan Mora<sup>1</sup>; Sangeet Adhikari<sup>1</sup>; Isabella Bonomi<sup>1</sup>; Purva Ranjan<sup>1</sup>; Alan Atkins<sup>2</sup>; Scott M Peterman<sup>2</sup>; Claudia Martins<sup>2</sup>; Philip Ma<sup>1</sup>; Bruce Wilcox<sup>1</sup>; <sup>1</sup>*PrognomiQ Inc, San Mateo, CA;* <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- ThP 789 **Unraveling Molecular Details Underlying COP9 Signalosome-mediated Regulation of Cullin-RING Ligases Using Quantitative Cross-linking Mass Spectrometry;** Xiaorong Wang<sup>1</sup>; Clinton Yu<sup>2</sup>; Fenglong Jiao<sup>2</sup>; Haibin Mao<sup>3</sup>; Ning Zheng<sup>3</sup>; Lan Huang<sup>2</sup>; <sup>1</sup>*University of*

## THURSDAY POSTERS

- California-Irvine, IRVINE, CA; <sup>2</sup>University of California Irvine, Irvine, CA; <sup>3</sup>University of Washington, Seattle, WA
- ThP 790 **TMTPro-18 utilized to decipher protein expression changes in synaptosomes in Post-Traumatic Stress Disorder (PTSD) as they relate to Opioid overdoses;** Katherine B Henke<sup>1, 2</sup>; Vena Martinez<sup>1</sup>; Weiwei Wang<sup>1, 2</sup>; Florine Collins<sup>1, 2</sup>; TuKiet T. Lam<sup>1, 2</sup>; Matthew Girgenti<sup>1</sup>; <sup>1</sup>Yale School of Medicine, New Haven, CT; <sup>2</sup>Keck MS & Proteomics Resource, New Haven, CT
- ThP 791 **Proteomic evaluation of tardigrades following ionizing radiation reveals increase in DNA repair pathways;** Evan R Stair<sup>1</sup>; Courtney Clark-Hatchel<sup>1, 2</sup>; Bob Goldstein<sup>1</sup>; Leslie M. Hicks<sup>1</sup>; <sup>1</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC; <sup>2</sup>University of North Carolina at Asheville, Asheville, NC
- ThP 792 **Absolute quantification of photoreceptor outer segment proteins;** Nikolai Skiba<sup>1</sup>; Tylor R. Lewis<sup>1</sup>; William J. Spencer<sup>2</sup>; Carson M. Castillo<sup>1</sup>; Andrej Shevchenko<sup>3</sup>; Vadim Y. Arshavsky<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC; <sup>2</sup>SUNY Upstate Medical University, Syracuse, NY; <sup>3</sup>Max Plank Institute of Molecular Cell Biology and Genetics, Dresden, Germany
- ThP 793 **Evaluating different recombinant Trypsin sequences for enhanced MS-based peptide identification and quantitative analysis;** Cristina Hernandez Rollan<sup>1</sup>; Tanveer Singh Batth<sup>1</sup>; Morten H. H. Nørholm<sup>2</sup>; Jesper Velgaard Olsen<sup>1</sup>; <sup>1</sup>Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark; <sup>2</sup>Novo Nordisk Foundation Center for Biosustainability, Denmark Technical University, Lyngby, Denmark
- ThP 794 **High-throughput LC-MS/MS enables protein Quantitative Trait Loci mapping in the progression of Metabolic Dysfunction-Associated Steatotic Liver Disease;** Margaret Lea Robinson<sup>1</sup>; Giorgia Benegiamo<sup>2</sup>; Jean-David Morel<sup>2</sup>; Wenyu Liu<sup>2</sup>; Katherine A Overmyer<sup>1, 3, 4</sup>; Johan Auwerx<sup>2</sup>; Joshua J Coon<sup>1, 3, 4, 5</sup>; <sup>1</sup>University of Wisconsin-Madison, Department of Biomolecular Chemistry, Madison, WI; <sup>2</sup>Laboratory of Integrative Systems Physiology, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; <sup>3</sup>Morgridge Institute for Research, Madison, WI; <sup>4</sup>National Center for Quantitative Biology of Complex Systems, Madison, WI; <sup>5</sup>University of Wisconsin-Madison, Department of Chemistry, Madison, WI
- ThP 795 **Extended Characterization and Multiplexed Quantification via a Chemical Proteomics Platform Using High-field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS);** Hung-Yu (Eric) Chiang<sup>1, 2</sup>; Min Ma<sup>1</sup>; Miyang Li<sup>3</sup>; Lingjun Li<sup>1, 3</sup>; <sup>1</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Biophysics Program, University of Wisconsin-Madison, Madison, Wisconsin; <sup>3</sup>Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- ThP 796 **Characterization of Proteins in Pig Sertoli Cells to Understand Complement System Behavior and Possible Xenotransplantation Applications Using LC-MS/MS Techniques;** Andrew I. Bennett<sup>1</sup>; Rachel Washburn<sup>2</sup>; Moyinoluwa Adeniyi<sup>1</sup>; Vishal Sandilya<sup>1</sup>; Jannette M. Dufour<sup>3</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>Ivy Tech Community College, Department of Life and Physical Sciences, Sellersburg, IN; <sup>3</sup>Texas Tech University Health Sciences Center, Lubbock, TX
- ThP 797 **Unleashing the Power of HT-DIA Acquisition on Orbitrap Exploris 240 – Precise and Accurate Quantitation at 260 SPD;** Maciej Bromirski<sup>1</sup>; Dominik Hoch<sup>2</sup>; Julia Kraegenbring<sup>3</sup>; Riccardo Stucchi<sup>2</sup>; Jeff Op De Beeck<sup>4</sup>; Robert Van Ling<sup>4</sup>; <sup>1</sup>Thermo Fisher Scientific, Warsaw, Poland; <sup>2</sup>Thermo Fisher Scientific GmbH, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>4</sup>Thermo Fisher Scientific, Ghent, Belgium
- ThP 798 **Innovative approaches for an in- depth quantitative analysis of the serum proteome of brown bears;** Alexandre GEFROY<sup>1</sup>; Hugo GIZARDIN-FREDON<sup>1</sup>; Jon ARNEMO<sup>2</sup>; Jonas KINDBERG<sup>3</sup>; Sarah CIANFERANI<sup>1</sup>; Guillemette GAUQUELIN-KOCH<sup>4</sup>; Lydie COMBARET<sup>5</sup>; Etienne LEFAL<sup>5</sup>; Fabrice BERTILE<sup>1</sup>; <sup>1</sup>Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, UMR 7178, ProFI FR2048, CNRS Université de Strasbourg, Strasbourg, France; <sup>2</sup>Inland Norway University of Applied Sciences, Koppang, Norway; <sup>3</sup>Norwegian Institute for Nature Research, Trondheim, Norway; <sup>4</sup>Centre National d'Etudes Spatiales, Paris, France; <sup>5</sup>Université Clermont Auvergne, INRAE, UNH UMR 1019, Clermont-Ferrand, France
- ThP 799 **Novel Hybrid Nominal Mass Instrument Enables Rapid Development of Large-Scale Targeted Plasma Proteomics Assays;** Yi (JIMMY) Zeng<sup>1</sup>; Philip M Remes<sup>2</sup>; Sangeet Adhikari<sup>1</sup>; Cristina C. Jacob<sup>2</sup>; Hao Qian<sup>1</sup>; Megan Mora<sup>1</sup>; Isabella Bonomi<sup>1</sup>; Purva Ranjan<sup>1</sup>; Alan Atkins<sup>2</sup>; Claudia Martins<sup>2</sup>; Philip Ma<sup>1</sup>; Bruce Wilcox<sup>1</sup>; <sup>1</sup>PrognomiQ Inc, San Mateo, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA

### SYSTEMS BIOLOGY 800-815

- ThP 800 **Cold skeletal muscle slices: A new approach to spatial visualisation of protein profiles;** Luisa Schmidt<sup>1, 2</sup>; Marcus Krüger<sup>1, 2</sup>; Philipp Antczak<sup>2, 3</sup>; Abigail Mackey<sup>4, 5</sup>; Christian Hoegsberg<sup>4, 5</sup>; Michael Saynisch<sup>2</sup>; <sup>1</sup>University of Cologne, Cologne, Germany; <sup>2</sup>CECAD (Cluster of Excellence in Cellular Stress Responses in Aging-Associated Diseases), Cologne, Germany; <sup>3</sup>CMMC (Center for Molecular Medicine), Cologne, Germany; <sup>4</sup>Institute of Sports Medicine Copenhagen, Copenhagen, Denmark; <sup>5</sup>University of Copenhagen, Copenhagen, Denmark
- ThP 801 **Shared peptides among diverse lineages of marine microeukaryotes;** Natalie Cohen<sup>1</sup>; Jaclyn K Saunders<sup>2</sup>; Mak A Saito<sup>3</sup>; <sup>1</sup>University of Georgia, Savannah, GA; <sup>2</sup>University of Georgia, Athens, GA; <sup>3</sup>Woods Hole Oceanographic Institution, Falmouth, MA
- ThP 802 **Illuminating the human phosphoproteome through the lens of clinical kinase inhibitors;** Florian P Bayer<sup>1</sup>; Julian Müller<sup>1</sup>; Matthew The<sup>1</sup>; Bernhard Kuster<sup>1, 2</sup>; <sup>1</sup>Technical University of Munich, Freising, Germany; <sup>2</sup>German Cancer Consortium (DKTK), Partner Site Munich, Munich, Germany
- ThP 803 **Data-Driven Modeling of the Mouse Macrophage Toll-like Receptor Signaling Pathway;** Nathan P. Manes<sup>1</sup>; Sergio A Hassan<sup>1</sup>; Anthony A Armstrong<sup>1</sup>; Fengkai Zhang<sup>1</sup>; Rachel A Gottschalk<sup>2</sup>; Matthew J Marino<sup>1</sup>; Iain DC Fraser<sup>1</sup>; Ronald N Germain<sup>1</sup>; Martin Meier-Schellersheim<sup>1</sup>; Aleksandra Nita-Lazar<sup>1</sup>; <sup>1</sup>National Institutes of Health, Bethesda, MD; <sup>2</sup>University of Pittsburgh, Pittsburgh, PA
- ThP 804 **Metabolite-protein architecture in the diversity outbred population defines mechanisms of control over metabolic pathways;** Haopeng Xiao<sup>1</sup>; Martha Ordonez<sup>1</sup>; Nils Burger<sup>1</sup>; Shelley M Wei<sup>2</sup>; Sumeet Khetarpal<sup>1, 3</sup>; Edward L. Huttlin<sup>4</sup>; Edward T Chouchani<sup>1</sup>; <sup>1</sup>Dana-Farber Cancer Institute/ Harvard Medical School, Boston, MA; <sup>2</sup>Dana-Farber Cancer Institute, Boston, MA; <sup>3</sup>MGH, Boston, MA; <sup>4</sup>Harvard Medical School, Boston, MA
- ThP 805 **Tumor ecosystem Interrogating via an multiomics strategy identifies novel therapeutic vulnerabilities for drug-resistant Acute Myeloid Leukemia patients;** Long Shen<sup>1</sup>; Yang Yang<sup>1</sup>; Chunliang Li<sup>2</sup>; Hong Wang<sup>1</sup>; <sup>1</sup>State key laboratory of blood science, Institute of Hematology & Blood Diseases Hospital, Chinese Academy of Medical Sciences & Peking Union Medical College, Tianjin, China; <sup>2</sup>St Jude Children's Research Hospital, Memphis, TN
- ThP 806 **High Throughput Simultaneous Multi-Omics Analysis by Direct Infusion Mass Spectrometry (SMAD-MS);** Yuming Jiang<sup>1</sup>; Ivan Salladay-Perez<sup>2</sup>; Amanda Momenzadeh<sup>1</sup>; Anthony J Covarrubias<sup>2</sup>; Jesse Meyer<sup>1</sup>; <sup>1</sup>Cedars-Sinai Medical Center, Los Angeles, CA; <sup>2</sup>University of California, Los Angeles, Los Angeles, CA
- ThP 807 **Synchrotron Radiolysis as Synthetic Reactive Oxygen Species Source Drives Methionine Sulfoxide Accumulation in ROS Sensitive E. coli Proteins.;** Ezaz Ahmed<sup>1, 2</sup>; Erik R. Farquhar<sup>1, 2</sup>; Daniela Schlatter<sup>3</sup>; Janna Kiselar<sup>2, 4</sup>; David T. Lodowski<sup>2, 4</sup>; Mark R. Chance<sup>1, 2, 4</sup>;

## THURSDAY POSTERS

<sup>1</sup>Center for Synchrotron Biosciences, Case Western Reserve University, School of Medicine, Cleveland, OH; <sup>2</sup>Department of Nutrition, Case Western Reserve University, School of Medicine, Cleveland, OH; <sup>3</sup>Center for Proteomics and Bioinformatics, Department of Nutrition, Case Western Reserve University, Cleveland, OH; <sup>4</sup>Center for Proteomics and Bioinformatics, Case Western Reserve University, School of Medicine, Cleveland, OH

- ThP 808 **Deciphering age-dependent global proteome changes in the leaf-cutting ant *Acromyrmex echinatior* for better understanding of biomineralization process;** Penghsuan Huang<sup>1</sup>; Joseph Sardina<sup>2</sup>; Haiyan Lu<sup>3</sup>; Cameron R. Currie<sup>2</sup>; Lingjun Li<sup>3</sup>; <sup>1</sup>University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Bacteriology, University of Wisconsin-Madison, Madison, WI; <sup>3</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, WI
- ThP 809 **The proteomic landscape of interferon signaling in primary human T cells and lung cells;** Christian M. Beusch<sup>1</sup>; Christopher Monaco<sup>1</sup>; David Ezra Gordon<sup>2</sup>; Samuel Gallant<sup>1</sup>; <sup>1</sup>Emory University School of Medicine, Atlanta, GA; <sup>2</sup>Emory University, Atlanta, GA
- ThP 810 **Formaldehyde crosslinking coupled RNA interactome capture at peptide-level enabled robust profiling of RNA-binding regions;** Seonmin Ju<sup>1,2</sup>; Yongwoo Na<sup>1,2</sup>; Jong-Seo Kim<sup>1,2</sup>; <sup>1</sup>School of Biological Sciences, Seoul National University, Seoul, South Korea; <sup>2</sup>Center for RNA Research, Institute of Basic Science (IBS), Seoul, South Korea
- ThP 811 **Global affinity-based organelle profiling reveals subcellular localization and remodeling at proteome scales;** Duo Peng<sup>1</sup>; Marco Y Hein<sup>1,2</sup>; Verina Todorova<sup>1</sup>; Frank McCarthy<sup>1</sup>; Kibeom Kim<sup>1</sup>; Chad Liu<sup>1</sup>; Laura Savy<sup>1</sup>; Camille Januel<sup>3</sup>; Rodrigo Baltazar-Nunez<sup>3</sup>; Sophie Bax<sup>1</sup>; Brian C DeFelice<sup>1</sup>; Shalin B Mehta<sup>1</sup>; Daniel N Itzhak<sup>3,4</sup>; Manuel D Leonetti<sup>1</sup>; Joshua E Elias<sup>1</sup>; <sup>1</sup>Chan-Zuckerberg Biohub, San Francisco, California; <sup>2</sup>Max Perutz Laboratories Vienna, Vienna BioCenter, Vienna, Austria; <sup>3</sup>Chan Zuckerberg Biohub, San Francisco, CA; <sup>4</sup>Altos Labs, Redwood City, California
- ThP 812 **Quantification of cell-type specific protein dynamics in *Drosophila* embryos;** Argit Marishta<sup>1</sup>; Martin Wühr<sup>1</sup>; Eric Wieschaus<sup>1</sup>; <sup>1</sup>Princeton University, Princeton, NJ
- ThP 813 **A subcellular proteome map of a marine organism using the Orbitrap Astral mass spectrometer;** Loay J. Jabre<sup>1</sup>; Matthew R. McIlvin<sup>1</sup>; Mak A. Saito<sup>1</sup>; <sup>1</sup>Woods Hole Oceanographic Inst., Woods Hole, MA
- ThP 814 **Evidence for widespread mesoscale cytoplasmic organization into condensates by quantitative proteomics of cell extract filtrates;** Felix C Keber<sup>1</sup>; Thao Nguyen<sup>1</sup>; Andrea Mariosi<sup>1</sup>; Clifford P Brangwynne<sup>1,2</sup>; Martin Wühr<sup>1</sup>; <sup>1</sup>Princeton University, Princeton, NJ; <sup>2</sup>Howard Hughes Medical Institute, Chevy Chase, MD
- ThP 815 **Deciphering hierarchical cell cycle controls with phosphoproteomics;** Anthony Cesnik<sup>1,2,3</sup>; Christian Gnann<sup>2,4</sup>; Frank McCarthy<sup>3</sup>; Daniel Itzhak<sup>3</sup>; Emma Lundberg<sup>1,2,3</sup>; <sup>1</sup>Stanford University, Stanford, CA; <sup>2</sup>KTH Royal Institute of Technology, Stockholm, Sweden; <sup>3</sup>Chan Zuckerberg Biohub, San Francisco, CA; <sup>4</sup>Chan-Zuckerberg Biohub, San Francisco, CA