POSTERS

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
7:00 - 8:00 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
7:00 - 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	136-156
Environmental: General	157-193
Environmental: Pharmaceuticals and Pesticides	194-207
Extractables & Leachables	208-218
Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements	219-237
Fundamentals: Ion Activation/Dissociation	238-248
Fundamentals: Ion Structure/Energetics/Reactions	249-264
Fundamentals: Molecular Modeling / Quantum Mechanical Calculations	265-270
Glycomics	271-296
H/D Exchange: Hardware, Software and Methodology	297-308
H/D Exchange: Protein Structure/Function	309-339
Imaging MS: Pharmaceuticals, Metabolites, Lipids, and Glycans I	340-364
Imaging: Spatially-Resolved Omics I	365-384
Industry: Trace Analysis, Quality Control, and Automation	385-394
Informatics: Metabolomics and Lipidomics	395-426
Informatics: Peptide ID and Quantification	427-457
Ion Mobility: Applications I	458-477
Lipids: ID and Structural Analysis I	478-497
Lipids: Profile Analysis	498-524
Metabolomics: General	525-556
Metabolomics: Untargeted Metabolite Profiling I	557-590
Microorganisms and the Microbiome I	591-615
Nucleic Acids and Oligonucleotides I	616-641
Peptides: Identification and Fragmentation Mechanisms	642-647
Peptides: PTM Identification	648-674
Process Development MS	675-686
Proteins: Complexes/Non-covalent Interactions	687-722
Proteomics: New Approaches I	723-742
Single Cell MS I	743-781
Small Molecules: Qualitative and Quantitative Analysis	782-804
Viruses and Virus-Like Particles	805-822

TUESDAY POSTERS

Set up all Tuesday posters
7:00 - 8:00 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
7:00 - 8:00 pm

Ambient Ionization: Applications II	001-021
Biomarkers: Quantitative Analysis I	022-048
Disease Biomarkers	049-063
Environmental: General II	064-099
Exposomics	100-118
Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements II	119-139
Fundamentals: Ion Molecule, Ion/Ion, Ion/Electron Interactions	140-156
Fundamentals: Native MS	157-173
High Throughput MS I	174-198
Imaging MS: Instrumentation	199-208
Imaging MS: Pharmaceuticals, Metabolites, Lipids, and Glycans II	209-231
Imaging: Spatially-Resolved Omics II	232-250
Informatics: Algorithms and Statistical Advances	251-287
Instrumentation: General	288-303
Ion Mobility: Applications II	304-323
Isotope Labeling and Fluxomics Applications	324-329
LC/MS: Sample Preparation I	330-350
Lipids: General	351-383
Lipids: ID and Structural Analysis II	384-403
Metabolomics: Clinical Applications	404-420
Metabolomics: Identification of Unknown Metabolites	421-433
Metabolomics: Sample Preparation	434-444
Metabolomics: Untargeted Metabolite Profiling II	445-478
Microorganisms and the Microbiome II	479-503
Nanoscale/Microfluidic and Capillary Electrophoresis Separations and MS	504-517
Neuroscience and Neurodegenerative Disease Research	518-539
Nucleic Acids and Oligonucleotides II	540-566
Peptidomics and Immunopeptidomics	567-596
Phosphopeptides and Phosphoproteins	597-617
Plant Biology and Biotechnology	618-629
Protein Therapeutics: Structural Characterization	630-659
Proteins: Conformation Analysis and Structural Biology	660-682
Proteomics: Chemoproteomics	683-715
Proteomics: Clinical Applications I	716-738
Proteomics: Infectious Diseases	739-743
Proteomics: New Approaches II	744-763
Single Cell MS II	764-783
Small Molecules: Qualitative and Quantitative Analysis II	784-805
Stable Isotope Labeling	806-820

POSTER OVERVIEW

WEDNESDAY POSTERS

Set up all Wednesday posters
7:00 - 8:00 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
7:00 - 8:00 pm

Ambient Ionization: Fundamentals and Instrumentation	001-008
Antibodies & Antibody Drug Conjugates I	009-039
Artificial Intelligence in MS Instrumentation and Applications I	040-065
Biomarkers: Discovery I	066-102
Biomarkers: Quantitative Analysis II	103-128
Cancer Research I	129-166
Clinical Analysis I	167-197
Covalent Labeling and Chemical Crosslinking I	198-223
Drug Discovery: Qualitative and Quantitative Analysis I	224-248
Environmental: General III	249-286
Fundamentals: Unconventional Approaches in MS	287-295
Glycoproteins I	296-326
High Throughput MS II	327-351
Imaging MS: Method Development I	352-385
Informatics: Protein ID and Quantification	386-398
Informatics: Workflow and Data Management	399-432
Instrumentation: Mini/Portable/Fieldable MS	433-444
Instrumentation: New Developments in Mass Analyzers and Ion Detection	445-460
Ion Mobility: FAIMS/DMS	461-467
Ion Mobility: General	468-481
LC/MS: Chromatography and Software	482-494
LC/MS: Sample Preparation II	495-514
Metabolomics: Targeted and Quantitative Analysis I	515-535
Neuroscience and Neurodegenerative Disease Research II	536-560
Nucleic Acids and Oligonucleotides III	561-587
Peptides: Targeted and Quantitative Analysis	588-618
Protein Therapeutics: Quantitative Analysis	619-643
Proteins: General and Membrane	644-659
Proteins: PTMs I	660-679
Proteomics: Intact Proteins and Top Down Analysis I	680-710
Proteomics: Quantitative I	711-745
Proteomics: Tissue	746-774
Single Cell MS III	775-796
Synthetic Polymers	797-810
Toxicology	811-823

THURSDAY POSTERS

Set up all Thursday posters
7:00 - 8:00 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
7:00 - 8:00 pm

Antibodies & Antibody Drug Conjugates II	001-033
Art, Archaeology & Paleontology	034-042
Artificial Intelligence in MS Instrumentation and Applications II	043-070
Biomarkers: Discovery II	071-100
Biomarkers: Quantitative Analysis III	101-127
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Clinical Analysis II	162-188
Covalent Labeling and Chemical Crosslinking II	189-213
Drug Discovery: Qualitative and Quantitative Analysis II	214-238
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Food Safety: General	246-274
Forensics	275-305
Fundamentals: Formation and Structures of Big Ions	306
Fundamentals: Ion Spectroscopy	307-311
Fundamentals: Ionic Clusters, Nanomaterials, and Catalysis	312-314
Fundamentals: Ionization	315-328
GC/MS: Instrumentation and Applications	329-367
Glycoproteins II	368-396
High Mass Accuracy/High Performance MS: Applications and Instrumentation	397-415
Imaging MS: Computational Methods, Software, and Analysis	416-432
Imaging MS: Disease Markers	433-445
Imaging MS: Method Development II	446-479
Informatics: General, SRM, and DIA	480-487
Informatics: Multiomics Integration	488-506
Instrumentation: New Concepts	507-523
Instrumentation: New Developments in Ionization and Sampling	524-542
Ion Mobility: Fundamentals	543-548
Ion Mobility: Structure	549-571
LC/MS: General	572-600
Lipids: Targeted and Quantitative Analysis	601-633
MALDI: Applications	634-644
MALDI: Innovation in Instrumentation and Sample Preparation	645-650
Metabolomics: Targeted and Quantitative Analysis II	651-672
Natural Products	673-700
Proteins: PTMs II	701-721
Proteomics: Clinical Applications II	722-743
Proteomics: Intact Proteins and Top Down Analysis II	744-772
Proteomics: Quantitative II	773-804
Systems Biology	805-824

MONDAY POSTERS

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7:00 - 8:00 pm

AMBIENT IONIZATION: APPLICATIONS
001-020

MP 001 **MS Imaging-Based Immunoscoring: Bringing Real-Time Intraoperative Prognosis to Life**; Léa LEDOUX[1]; Yanis Zirem[1]; Lucas Roussel[1]; Bertrand Meresse[2]; Michel Salzet[1]; Isabelle Fournier[1]; *[1]PRISM Inserm U1192 - University of Lille, Villeneuve d'Ascq Cedex, France; [2]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[1]; Stefan J Swift[2]; Patrik Španěl[3]; Kseniya Dryahina[3]; Mark J. Perkins[4]; Vaughan S. Langford[5]; *[1]Syft Technologies, Los Angeles, CA; [2]University of Oslo, Oslo, Norway; [3]J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic; [4]Element Lab Solutions, Cambridge, United Kingdom; [5]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[1]; Terry L Bates[1, 2]; Brett L Bergman[1]; Gavin L Sacks[1]; *[1]Cornell University Dept. of Food Science, Ithaca, NY; [2]Bruker Daltonics Inc., Billerica, MA*

MP 004 **SICRIT-HRMS for Metabolic Profiling through Direct Breath Analysis**; Ciara Conway[1, 2]; Taylor Hayward[3]; Jan-Christoph Wolf[2]; Christoph Haisch[1]; *[1]Technical University of Munich (TUM), Munich, Germany; [2]Plasmion GmbH, Augsburg, Germany; [3]Plasmion, Skillman, NJ*

MP 005 **Where did that come from? Non-targeted identification of micro-scale contaminants with laser desorption ionization methods**; Andre Benally[1]; Jessica K Kustas[1]; Ryan D. Davis[1]; *[1]Sandia National Laboratories, Albuquerque, NM*

MP 006 **DART-MS Analysis of Antiparasitic Compounds in Bovine Hair, a powerful tool**; Almir Custódio Batista Junior[1]; Lanaia Louzeiro Maciel[1]; Yuri Arrates Rocha[1]; Gabriela G Souza[1]; Marc I Chalon[2]; Boniek Gontijo Vaz[1]; Welber Daniel Z Lopes[1]; Ana Flávia M. Botelho[1]; Andrea Rodrigues Chaves[3]; *[1]Universidade Federal de Goiás, Goiânia, Brazil; [2]SENS Advanced Mass Spectrometry, São Paulo, Brazil; [3]Universidade Federal de Goiás, Goiânia, Brazil*

MP 007 **Model reference library of mass spectrometry profiles for analysis of autopsy material**; Stanislav Pekov[1, 2, 3]; Andrey Temnov[2]; Ekaterina Parochkina[2]; Mikhail Oliferenko[2]; Olga Dorovatovskaya[2]; Igor Popov[2, 3]; *[1]Skolkovo Institute of Science and Technology, Skolkovo, Russia; [2]Moscow Institute of Physics and Technology, Dolgoprudniy, Russian Federation; [3]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[1]; Josiah McKenna[1]; Connor Moreillon[1]; Chengli Zu[1]; *[1]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[1]; Lauren Katz[2]; Lan Anna Ye[1]; Georgia Gopinath[2]; Taira Kiyota[3]; Claudia Kuzan-Fischer[4]; Mark Zaidi[2]; Kaitlyn Peters[2]; Ahmed Aman[3]; Trevor McKee[1]; Fred Fu[1]; Siham Amara-Belgadi[2]; Craig Daniels[4]; Brad Wouters[1]; James Rutka[4]; Howard Ginsberg[5]; Chris McIntosh[2]; Arash Zarrine-Afsar[2]; *[1]University Health Network, Toronto, ON; [2]University of Toronto, Toronto, ON; [3]Ontario Institute for Cancer Research, Toronto, ON; [4]The Hospital for Sick Children, Toronto, ON; [5]Unity Health Toronto, St Michael's Hospital, Toronto, Ontario*

MP 010 **In SituDerivatization of Unsaturated Mid-Chain Alcohols with Pyridine during Direct Analysis in Real Time Mass Spectrometry (DART-MS)**; Zoë Scott[1]; Andre P Kalenak[2];

Gavin L Sacks[2]; [1]*Cornell University, Ithaca, NY;* [2]*Cornell University Dept. of Food Science, Ithaca, NY*

MP 011 **Portable Mass Spectrometer with Dielectric Barrier Discharge Ionization for the Direct Analysis of Controlled Substances and Explosives**; Taylor Hayward[1]; Krisztian Torma[2]; William Yang Terziyan[2]; Jan Bucek[3]; Jan-Christoph Wolf[3]; [1]*Plasmion, Skillman, NJ;* [2]*BaySpec, Inc, San Jose, CA;* [3]*Plasmion GmbH, Augsburg, Germany*

MP 012 **Elucidating the Formose Reaction in aqueous microdroplets via Nano-Electrospray Ionization Mass Spectrometry**; Myles Edwards[1]; Dylan T. Holden[2]; R. Graham Cooks[2]; [1]*Purdue University, West Lafayette, IL;* [2]*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[1]; Xiaokun Duan[1]; Charles C. Liu[1]; [1]*ASPEC Technologies, Suzhou, China*

MP 015 **Detecting chemical threats with minimal sample preparation and without chromatographic separation**; HJ Jost[1]; Fariba Partovi[1, 2]; Joona Mikkilä[1]; Jyri Mikkilä[1]; Jussi Kontro[1]; Paxton Juuti[1]; Aleksei Shcherbinin[1]; [1]*Karsa Ltd, Helsinki, Finland;* [2]*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[1]; Pingping Wang[1]; Lei Li[1]; Junliang Zhang[1]; [1]*Ningbo University, Ningbo, China*

MP 017 **Rapid Screening and Quantification of PFAS in Contaminated Soil utilizing DART-MS/MS**; Zahuindanda Aventura[1]; Gregory Nieckarz[1]; [1]*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[1]; Yu Ning Shiu[2]; Frederick W Woodley[3]; Abraham K. Badu-Tawiah[1]; [1]*The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio;* [2]*The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH;* [3]*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[1]; Hsin-Bai Zou[2]; Wei-Kai Wu[3]; Cheng-Chih Hsu[1, 2]; [1]*Department of Chemistry, National Taiwan University, Taipei, Taiwan;* [2]*Leeuwenhoek Laboratories Co. Ltd., Taipei, Taiwan;* [3]*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*

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[1]; Yvonne Wu[1]; Brian Agan[1]; Jennifer Gogley[1]; [1]*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[1]; Insa Peters[2]; Ann-Marie Garzinsky[1, 3]; Lina Lucuta[4]; Martin Juebner[4]; Nana Naumann[2]; Mikael Hedeland[3]; [1]*German Sport University, Cologne, Germany;* [2]*Manfred-Donike Institute for Doping Analysis, Cologne, Germany;* [3]*Uppsala University, Uppsala, Sweden;* [4]*University of Cologne, Cologne, Germany*

MP 023 **Quantification of Δ9-THC and their isomers in Cannabis-based drug matrices by UHPLC-MS**; Hildegardo Seibert Franca[1, 2, 3]; João Victor De Almeida[2, 3]; Nayara A. dos Santos[2, 3]; Nathália Conceição[2, 3]; Marcos Valério V. Lyrio[2, 3]; Alan Reink Pereira[2, 3]; Wanderson Romao[1, 2, 3]; [1]*Federal Institute of Espírito Santo, Brazil, Vila Velha, Brazil;* [2]*National Institute of Forensic Science and Technology, INCT, Porto Alegre, Brazil;* [3]*Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espirito 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[1]; Kelsey L Abbott[1]; Benjamin J Burris[1]; Soobeng Tan[1]; [1]*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[1]; Fabio Comunità[1]; Xavier De La Torre[1]; Francesca Terracciano[1]; Francesco Botre[1]; [1]*Laboratorio Antidoping FMSI, Roma, Italy*

MP 026 **Detection of Perfluorocarbons in Equine Blood via Headspace GC-MS/MS**; Leif K. McGoldrick[1, 2]; Fuyu Guan[1, 2]; Mary A. Robinson[1, 2]; [1]*Department of Clinical Studies – New Bolton Center, School of Veterinary Medicine, University of Pennsylvania, Kennett Square, PA;* [2]*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[1, 2]; Youwen You[1, 2]; Jaclyn R. Missanelli[1, 2]; Kacee Rossi[1, 2]; Katelyn Stalker[1, 2]; Mary A. Robinson[1, 2]; [1]*University of Pennsylvania School of Veterinary Medicine, Pennsylvania, PA;* [2]*Pennsylvania Equine Toxicology & Research Laboratory, West Chester, Pennsylvania*

MP 028 **Comprehensive analysis of minor hemp cannabinoids with therapeutic potential**; Jaewoo Choi[1]; Parker Rianda[2]; Inah Gu[3, 4]; Claudia S. Maier[1, 3]; Jan F. Stevens[3, 4, 5]; [1]*Department of Chemistry, Oregon State University, Corvallis, OR;* [2]*Bioresources Research Program, College of Agricultural Sciences, Oregon State University, Corvallis, OR;* [3]*Linus Pauling Institute, Oregon State University, Corvallis, OR;* [4]*Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR;* [5]*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[1]; Brandon L. Salazar[2]; Jill Hochreiter[2]; Jill Lapham[2]; Stephen Ross[3]; Troy D. Wood[1]; Gene D. Morse[2]; [1]*Department of Chemistry, Natural Sciences Complex, University at Buffalo, State University of New York, Buffalo, NY;* [2]*Department of Pharmacy Practice, School of Pharmacy and Pharmaceutical Sciences, NYS Center for Integrated Global Biomedical Sciences, Translational Pharmacology Research Core, Buffalo, NY;* [3]*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[1]; Hyeon-Jeong Lee[1]; Yoodam Seo[1]; Hophil Min[1]; [1]*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[1]; Isabel V C Fulchini[2]; Joice R Dos Santos[2, 3];

Marcos A Pudenzi[1]; Diogo Oliveira-Silva[2]; Ichiro Hirano[1]; *[1]Shimadzu do Brasil, Barueri, Brazil; [2]Universidade Federal de Sao Paulo, DIadema, Brazil; [3]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[1]; Andrew M. Pritchard[1]; Michael S. Cordes[1]; Elyssia S Gallagher[1]; *[1]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[1]; Ron Orlando[2]; *[1]University of Georgia - Complex Carbohydrate Research Center, Athens, GA; [2]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[1, 2]; Christopher Ashwood[1, 2, 3]; Lukas Muerner[1, 4]; Richard D. Cummings[1, 2]; *[1]Beth Israel Deaconess Medical Center, Boston, MA; [2]Harvard Medical School, Boston, MA; [3]Protea Glycosciences, Sydney, Australia; [4]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[1]; Zachary Hartman[1]; Anton N. Kozhinov[2]; Konstantin Nagornov[2]; Eric Lafontaine[1]; Jeff Hogan[1]; Daniel G Mead[1]; Yury Tsybin[2]; Franklin E. Leach III[1]; *[1]University of Georgia, Athens, GA; [2]Spectroswiss, Lausanne, Switzerland*

MP 036 **From Fragments to Frameworks: Characterization of Marine Polysaccharide Structures using MS-based Multi-Platforms**; Nari Seo[1, 2]; Hyun Joo An[1, 2]; *[1]Chungnam National University, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea*

MP 037 **Distinguishing Co2+-Adducted Anomeric Carbohydrate Isomers with HCD, ETD, and EThcD** ; Andrew Pritchard[1]; Darren T. Gass[1]; Elyssia S Gallagher[1]; *[1]Baylor University, Waco, TX*

MP 038 **Capillary Zone Electrophoresis - Mass Spectrometry and Statistics Analysis of Plasma Chondroitin Sulphate Oligosaccharides in Septic Patients**; Yiqing Zhang[1]; I. Jonathan Amster[2]; *[1]University of Georgia, Department of Chemistry, Athens, GA; [2]University of Georgia, Athens, GA*

MP 039 **Development of High Sensitivity MS Methods for Identification and Quantification of Glycosphingolipids (GSLs)**; Mehrnoush Taherzadeh Ghahfarrokhi[1]; Stephanie Archer-Hartmann[1]; Christian Heiss[1]; Parastoo Azadi[1]; *[1]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[1]; Alexander E. Toler[1]; Jody C. May[1]; John A. McLean[1]; *[1]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[1]; Yat Ming So[1]; Fred K. W. Kong[1]; David K. K. Leung[1]; April S. Y. Wong[1]; Wai Him Kwok[1]; Terence S. M. Wan[1]; Emmie N. M. Ho[1]; *[1]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[1]; Doeun Kim[1]; Gwang Bin Lee[2]; Ling Hao[2]; Aleksandra Nita-Lazar[1]; *[1]NIH/NIAID, Bethesda, MD; [2]The George Washington University, Washington, DC*

MP 043 **Pushing the boundaries of sensitivity and depth-of-coverage for nanoflow proteomics**; Katherine Tran[1]; Ihor Batruch[1]; Stephen Tate[1]; Patrick Pribil[1]; *[1]SCIEX, Concord, ON*

MP 044 **SWATH-MS analysis of butyric acid effect on mAbs production and redox homeostasis in CHO cells**; Mauro Galli[1]; Yee Jiun Kok[1]; Xuezhi Bi[1, 2, 3]; *[1]A-Star, Bioprocessing Technology Institute, Singapore, Singapore; [2]Duke-NUS Medical School, Singapore, Singapore; [3]Singapore Institute of Technology, Singapore, Singapore*

MP 045 **Targeted quantitative screening pesticides in food matrices using high resolution DIA spectral library matching**; Alan Barnes[1]; Raquel Leonardo[2]; Emily G Armitage[1]; Jonathan McGeehan[3]; Steve Williams[2]; Neil J Loftus[1]; *[1]Shimadzu Corporation, Manchester, United Kingdom; [2]SGS Cambridge Limited, Cambridge, United Kingdom; [3]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[1]; Pauline Perdu-Alloy[1]; Charline Keller[1]; Christine Schaeffer[1]; Christine Carapito[1]; *[1]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[1]; Hem Gurung[2]; Amanda Lorentzian[2]; Fengchao Yu[3]; Meena Choi[2]; Ying Zhu[2]; *[1]Genentech Inc., South San Francisco, CA; [2]Genentech Inc, South San Francisco, CA; [3]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[1]; Sung-Fang Chen[2]; *[1]National Taiwan Normal University, Taipei, Taiwan; [2]National Taiwan Normal University, Taipei, Taiwan*

MP 049 **Protein Quantification Assessment of diaPASEF Mode on timsTOF SCP**; Ju Wang[1]; Haiyan Tan[1]; Yingxue Fu[1]; Ashutosh Mishra[1]; Huan Sun[1]; Zhen Wang[1]; Zhiping Wu[1]; Xusheng Wang[1]; Junmin Peng[1]; Anthony High[1]; *[1]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[1]; Julia Kraegenbring[2]; Julian Saba[3]; Maciej Bromirski[4]; Amirmansoor Hakimi[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, Winnipeg, MB; [4]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[1]; Sebastian V Jacome[2]; Nhi Ngo[1]; Radu M Suciu[1]; Matthew Willetts[3]; Micah J Niphakis[1]; *[1]Lundbeck, San Diego, CA; [2]Bruker Scientific, 40 Manning Road, Billerica, MA; [3]Bruker Scientific, LLC, Billerica, MA*

MP 053 **Deep Proteomic Profiling of Accelerated Kidney Aging and Senescence Burden in Macaca mulatta**; Christina D King[1]; Jordan B Burton[1]; George Schaaf[2]; Stephen Kritchevsky[2]; J. Mark Cline[2]; Jamie N Justice[2, 3]; Ellen E Quillen[2]; Birgit Schilling[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]Wake Forest University School of Medicine, Winston-Salem, NC; [3]XPRIZE Foundation, Culver City, CA*

MP 054 **Database search result comparison for Spectronaut and DIANN for DIA data collected from QE, Fusion, Eclipse, Exploris and TimsTOF Pro2**; Dennis Province[1]; Stephanie Byrum[1]; Michael Kinter[2]; Ricky Edmondson[1]; Samuel Mackintosh[1]; Alan Tackett[1]; *[1]UAMS, Little Rock, AR; [2]Oklahoma Medical Research Foundation, Oklahoma City, Oklahoma*

MP 055 **Improved proteome coverage combined with reproducible quantitation on the timsTOF platform**; Dijana Vitko[1]; Stephanie Kaspar-Schoenefeld[2]; Andreas Schmidt[2]; Markus Lubeck[2]; Pierre-Olivier Schmit[3]; Torsten Mueller[2]; *[1]Bruker Daltonics GmbH & Co. KG, Billerica, MA; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [3]Bruker France SAS, Wissembourg, France*

MP 056 **A scanning DIA workflow for quantitative LC-MS/MS with minimal method development**; Anjali Chelur[1]; Gordana Ivosev[1]; Nic G Bloomfield[1]; Claudia Alvarez[1]; Stephen Tate[1]; *[1]SCIEX, Concord, ON*

MP 057 **Synchronizing analysis with acquisition for significantly faster library free analysis of DIA**; Damiano Robbiani[1]; Grzegorz Skoraczyński[1]; Oliver M. Bernhardt[1]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

MP 058 **High-throughput cancer proteomic characterization using data-independent mass spectrometry (DIA-MS)**; Chih-Hsuan Yeh[1, 2]; Sebastian P. Perner[1, 3]; Yanlong Ji[1, 2]; Silvia Münch[3]; Thomas Oellerich[3]; Kuan-Ting Pan[1]; Henning Urlaub[1, 2]; *[1]Bioanalytical Mass Spectrometry Group, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; [2]Bioanalytics Group, Institute of Clinical Chemistry, University Medical Center Göttingen, Göttingen, Germany; [3]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[1]; Amarjeet Flora[2]; Bhavin Patel[2]; Santosh Renuse[3]; Ryan Bomgarden[2]; Nicolaie Eugen Damoc[1]; *[1]Thermo Fisher Scientific GmbH, Bremen, Germany; [2]Thermo Fisher Scientific, Rockford, Illinois; [3]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[1]; Alexander Hogrebe[1]; Daniel P Zolg[1]; Florian Seefried[1]; Martin Frejno[1]; *[1]MSAID, Garching, Germany*

MP 062 **Trapped Ion Mobility Separation (TIMS) in Combination with Scanning Quadrupole Isolation for Data Independent Acquisition in Proteomics**; Markus Lubeck[1]; Eike Mucha[1]; Stephanie Kaspar-Schoenefeld[1]; Christoph Krisp[1]; Andreas Schmidt[1]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

MP 063 **DIA analysis of Nrf2 and αB-crystallin mutant zebrafish lenses under oxidative stress**; Sarah Zelle[1]; Hassane S. Mchaourab[1]; Kevin L. Schey[1]; *[1]Vanderbilt University, Nashville, TN*

MP 064 **Quantitative and Qualitative Evaluation Performance of diaPASEF for Targeted Protein Degradation**; Duc Tran[1]; Shu You[1]; Alex Campos[1]; *[1]Plexium, San Diego, CA*

MP 065 **Quantifying the Benefits of Using Study-Specific Data-Independent Acquisition Libraries for Proteomics Analysis**; Mynaja Ferguson[1]; Dorianne Robasson[2]; Rachel Muriph[1]; Kai Zou[1]; Hannah Rosen[2]; Jason Evans[2]; *[1]Univeristy of Massachusetts Boston, Boston, MA; [2]University of Massachusetts Boston, Boston, MA*

MP 066 **Direct, spectrum-centric peptide identification from diaPASEF data**; Kai Li[1]; Fengchao Yu[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, Michigan*

MP 067 **Data independent acquisition (DIA) for peptide library generation prior to HDX-MS**; Oliver Wu[1]; Joel B Langford[1]; Kellye Cupp-Sutton[2]; Nathan Basisty[3]; Si Wu[2]; *[1]University of Oklahoma, Norman, OK; [2]University of Alabama, Tuscaloosa, AL; [3]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[1]; Morgan Fair[1]; Liang Zhao[1]; Qing Wang[1]; *[1]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[1]; Wenxue Li[1]; Yi Di[1]; Diego Assis[2]; Matthew Willetts[2]; Yansheng Liu[1]; *[1]Yale University, West Haven, CT; [2]Bruker life sciences, Billerica, MA*

MP 070 **Evaluating mass spectrometry strategies for deep proteome profiling with subcellular fractionation**; Andrea I Gutierrez[1]; Julia E Robbins[1]; J. Sebastian Paez[1]; Tonibelle Gatbonton-Schwager[1]; Alexander J Federation[1]; Daniele Canzani[1]; Lindsay K Pino[1]; *[1]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[1]; Avinash Singh[1]; Sanjeeva Srivastava[1]; *[1]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[1]; Samuel L Arnold[1]; *[1]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[1]; Julia Kraegenbring[2]; Julian Saba[3]; Amanda E Lee[4]; Tonya Pekar-Hart[1]; Jingjing Huang[1]; Amirmansoor Hakimi[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermo Fisher Scientific, Winnipeg, MB; [4]Thermo Fisher Scientific, Worcester, MA*

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MP 074 **Developing a Targeted LC-HRMS Workflow for Quantifying Transporter Proteins in Complex In-vitro System**; Danqing Wang[1]; Yusi Cui[1]; Yuling Dai[2]; Benjamin Lai[1]; Qinying Yu[1]; Eugene Chen[1]; Xing Zhang[1]; *[1]Genentech Inc, South San Francisco, CA; [2]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[1]; Christopher Rowbottom[1]; John Wickwire[1]; Mark Brader[1]; Ling Morgan[1]; *[1]Moderna, Cambridge, MA*

MP 076 **Identifying and Assessing Target Engagement of Ligands Binding to Activin Ligand Traps**; Mark Athanason[1]; Keun-Joong Lee[1]; Matthew Mazur[1]; Yan Gao[1]; Richard Chen[1]; *[1]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[1]; Franck Amblard[1]; Selwyn Hurwitz[1]; Mahesh Kasthuri[1]; Chengwei Li[1]; Julia LeCher[1]; Junxing Shi[1]; Ramyani De[1]; Jessica Bowen-Downs[1]; Raymond Schinazi[1]; *[1]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[1, 2]; Nour Bou Karroum[3]; Catherine Piveteau[3]; Aurore Tomezyk[1]; Julie Dumont[3]; Mathieu Gaudin[1]; Rebecca Deprez-Poulain[2, 3]; Corinne Ramos[1, 2]; Benoit Deprez[3]; *[1]Aliri, Loos, France; [2]CAPSTONE-ETN MSCA network, Lille, France; [3]Drugs and Molecules for Living Systems, U1177, Lille, France*

MP 079 **Accurate Identification of Phase I Oxidative Metabolites of the Proteolysis Targeting Chimera (PROTAC™)**

Degrader GNE-987; Pengyi Hou[1]; Dandan Si[1]; Zhimin Long[1]; Lihai Guo[1]; *[1]SCIEX, Beijing, China*

MP 080 **Enhancement of Sensitivity and Quantification Quality in the LC-MS/MS Measurement of Large Biomolecules with Sum of MRM (SMRM)**; Liang Tang[1]; Robert R. Swezey[1]; Carol E. Green[1]; Jon C. Mirsalis[1]; *[1]SRI International, Menlo Park, CA*

MP 081 **Labeling of lipopeptides with lanthanide tag enables their monitoring in biological tissues by ICP-MS**; Aneta Myskova[1, 2]; Antonín Kaňa[1]; Tomáš David[2]; David Sýkora[1]; Miloslav Polášek[2]; Miroslava Šedinová[2]; Jaroslav Kuneš[3]; Lenka Maletínská[2]; *[1]University of Chemistry and Technology Prague, Prague, Czech Republic; [2]Institute of Organic Chemistry and Biochemistry, CAS, Prague, Prague, Czech Republic; [3]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[1]; Sarah Franc[1]; Bocheng Yin[1]; Fletcher Paddison[1]; Gyana Cureg[1]; Fabio Broccatelli[1]; *[1]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[1]; Suraj Dhungana[2]; Robert Plumb[2]; Amy Bartlett[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]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[1]; Jeong-hyeon Lim[1]; Sangsoo Hwang[1]; Yuna Shin[2]; Hyunjin Kim[2]; Seunghyun Jo[2]; Duckhyang Shin[2]; Sang Ho MA[2]; Myung L. Kim[2]; Young G. Shin[1]; *[1]College of Pharmacy and Institute of Drug Research and Development, Chungnam National University, Daejeon, South Korea; [2]Bilix Co., Ltd., Yongin, South Korea*

MP 085 **Bioanalytical Method Development and its Application to Pharmacokinetic Characterization of Tramiprosate and ALZ-801**; Jeonghyeon Lim[1]; Jeongmin Lee[2]; Seo-jin Park[2]; Sang-soo Hwang[2]; Eun-jeong Jo[2]; Young G. Shin[2]; *[1]Chungnam National Univeristy, Daejeon, South Korea; [2]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[1]; Annie Run Qi Shao[1]; Linh Nguyen[1]; Harun Rashid[1]; William Donaldson[2]; *[1]Nuchem Sciences Inc., Montréal, QC; [2]Estrigenix Therapeutics, Milwaukee, WI*

MP 087 **Utilization of CID and EAD fragmentation for metabolite identification in three hepatocyte models**; Yiran Huang[1]; Bennett K Ma[1]; Amy G Aslamkhan[1]; *[1]Merck Sharp & Dohme LLC, West Point, PA*

MP 088 **Ultra-Performance Liquid Chromatography-Tandem Mass Spectrometry Method Development and Pharmacokinetics of 10β,17β-Dihydroxyestra-1,4-dien-3-one (DHED) in Mice**; Amy Q Wang[1]; China Ryu[1]; Elias Padilha[1]; Patrick J. Morris[1]; Abagail F Postle[2]; Chris F Powels[2]; Todd D Gould[2]; Xin Xu[1]; *[1]NIH, Rockville, MD; [2]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[1]; Seo-jin Park[1]; Jeong-hyeon Lim[1]; Young G. Shin[1]; *[1]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[1]; Maria Fawaz[1]; Mark T. Cancilla[1]; Raymond Gonzalez[1]; Kara M Pearson[1]; Yu Feng[1]; *[1]Merck & Co. Inc., West Point, PA*

MP 091 **Beyond Western Blot: LC-MS Revolutionizes Protein Analysis with Speed and Precision**; Dhaval Patel[1]; Yash Mehta[1]; Ulrich Bickel[1]; Abraham Al-Ahmad[1]; *[1]Texas Tech University Health Sciences Center, Amarillo, TX*

MP 092 **Evaluation of BioMimetic Oxidation Kit for Fast and Efficient Abiotic Metabolite Generation**; Rong Chen[1]; Vivek Badwaik[1]; Jesse Balcer[1]; Chengli Zu[1]; *[1]Corteva Agriscience, Indianapolis, IN*

MP 093 **Proteomic-Based Site-Specific Covalent Ligand Screening for FBDD-Driven PROTAC Development Targeting MDM2**; Hyeonjun Lee[1]; Ju Yeon Lee[2]; Minhee Kang[1]; Suin Kim[1]; Jaebong Jang[1]; Jin Young Kim[2]; Young Ho Jeon[1]; *[1]College of Pharmacy, Korea University, Sejong, South Korea; [2]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[1]; Yuetian Yan[1]; Shunhai Wang[1]; Ning Li[1]; *[1]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[1]; Loren Olson[2]; Jamie Jorski[1]; Christopher Chhin[1]; Wayne Lootsma[3]; Steve Ainley[3]; Jeremy Lawton[3]; Laurent Salphati[1]; *[1]Genentech Inc, South San Francisco, CA; [2]SCIEX, Redwood City, CA; [3]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[1]; Jeffrey J. Jacson[1]; Iain D.G. Campuzano[1]; Rahul Baghla[2]; *[1]Amgen Inc., Thousand Oaks, CA; [2]SCIEX, Redwood City, CA*

MP 100 **Doping Control of Estra-4,9-diene-3,17-dione in horses**; Helen S.M. Ho[1]; Adrian F. Farrington[2]; Amanda J. Bond[3]; Emmie N. M. Ho[1, 4]; Wing-Tak Wong[1]; *[1]The Hong Kong Polytechnic University, Hong Kong, Hong Kong; [2]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; [3]Equestrian Affairs, The Hong Kong Jockey Club, Sha Tin Racecourse, Sha Tin, N. T., Hong Kong, China, Hong Kong, China, Hong Kong; [4]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[1]; Firoz Khan[1]; Huzefa Raja[1]; Cedric Pearce[2]; Shabnam Hematian[1]; Nicholas Oberlies[1]; *[1]UNCG, Greensboro, NC; [2]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 spectraometry**; Peng Li[1]; Ya Ding[1]; Lian Guo[1]; Lingling Zhang[1]; Weiqun Cao[1]; Yi Tao[1]; Liang Shen[1]; *[1]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[1]; Ju-Hyun Kim[1]; *[1]Yeungnam University, Gyeongsan-si, South Korea*

MP 104 **Elucidation of Isomeric Metabolites of Cyclic Peptide PharmaceuticalsUsing HPLC/ESI-Exact-Mass-MS/MS Data with MASSPEC Structure Elucidation Software**; Marshall M. Siegel[1]; Serhiy Hnatyshyn[2]; Gary Walker[1]; [1]*MS Mass Spec Consultants, Fair Lawn, NJ;* [2]*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[1]; Donald Chun[1]; Veronica Viramontes[1]; Zhili Li[1]; David Cipolla[1]; [1]*Insmed, Bridgewater Township,, NJ*

MP 106 **Metabolite identification of the targeted protein degrader, ARV-110**; Junmiao Chen[1]; Dandan Si[1]; Zhimin Long[1]; Lihai Guo[1]; [1]*SCIEX, Beijing, China*

MP 107 **Benefits of DIA for metabolism studies**; Stephen Tate[1]; Chris Brown[2]; Jeffrey R Gilbert[2]; Yves LeBlanc[1]; [1]*SCIEX, Concord, ON;* [2]*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[1]; Magdalena Vagnerova[2, 3]; Monika Mrnava[1]; Petr Palivec[1]; Martin Kuchar[1]; [1]*Forensic Laboratory of Biologically Active Substances, Department of Chemistry of Natural Compounds, University of Chemistry and Technology Prague, Prague 6, Czech Republic;* [2]*Forensic Laboratory of Biologically Active Substances, Department of Chemistry of Natural Compounds, University of Chemistry and Technology, Prague, Czech Republic;* [3]*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[1]; Felix Schumacher[1]; Kerstin Hofer[2]; Mads Mansoe[3]; Christian Weile[3]; Erich Koller[1]; Sabine Lohmann[2]; Sabine Schuster[2]; Andreas Brink[1]; [1]*Pharma Research and Early Development, Roche Innovation Center Basel, Basel, Switzerland;* [2]*Pharma Research and Early Development, Roche Innovation Center Munich, Penzberg, Germany;* [3]*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[1]; Wencui Yin[1]; Adnan A Kadi[1]; [1]*King Saud University, Riyadh, Saudi Arabia*

MP 111 **High-Throughput Screening and Proteomic Characterization of Compounds Targeting Myeloid-Derived Suppressor Cells**; Johannes Krumm[1, 2]; Elissaveta Petrova[3]; Severin Lechner[2]; Julia Mergner[2]; Hans-Henning Boehm[3]; Alessandro Prestipino[3]; Dominik Steinbrunn[1]; Marshall L. Deline[4]; Hannes Hahne[1]; Jan-Carsten Piek[3]; Bernhard Kuster[2]; [1]*OmicScouts GmbH, Freising, Germany;* [2]*Chair of Proteomics and Bioanalytics, TU Munich, TUM School of Life Sciences, Freising, Germany;* [3]*Merck KGaA, Darmstadt, Germany;* [4]*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[1]; Giovanni Andrea Vitale[2]; Steffen Heuckeroth[1]; Daniel Petras[2, 3]; Uwe Karst[1]; [1]*University of Muenster, Muenster, Germany;* [2]*University of Tuebingen, CMFI Cluster of Excellence, Interfaculty Institute of Microbiology and Infection Medicine, Tübingen, Germany;* [3]*UC Riverside, Riversdie, CA*

MP 113 **Application of LC-HRMS for metabolic studies of hexahydrocannabinol (HHC) using Cunninghamella elegans mycelia and Wistar rat models** ; Monika Mrnava[1]; Magdalena Vagnerova[1, 2]; Lucie Janeckova[1]; Martin Kuchar[1]; Petr Palivec[1]; Bronislav Jurasek[1]; [1]*Forensic Laboratory of Biologically Active Substances, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic;* [2]*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[1]; Min Du[2]; [1]*Thermo Fisher Scientific, San Jose, CA;* [2]*Thermo Fisher Scientific, Lexington, MA*

MP 115 **Simultaneous Quantitation of Prednisone and Prednisolone in Human Plasma by LC-MS/MS**; Moo-Young Kim[1]; Xuguang Yan[1]; Weijun Sun[1]; Zhijing Huang[1]; Melissa Mofikoya[1]; [1]*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[1]; Hania Khoury-Hollins[2]; Ismael Zamora[3]; Fabien Fontaine[3]; Michael McCullagh[2]; Martin Palmer[2]; Richard Lock[2]; Laura Tomlinson[1]; Leah Bottomley[1]; Richard Gregory[1]; [1]*GSK, Stevenage, United Kingdom;* [2]*Waters Corporation, Wilmslow, United Kingdom;* [3]*Mass Analytica Ltd, Sant Cugat del Vallés, Spain*

MP 117 **The Automated Sample Preparation Workflow and Toolbox for Bioanalysis**; Yuan Li[1]; Kyle Dukes[1]; Amber Cain[1]; Esraa AboJasser[1]; [1]*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[1]; Steffen Heuckeroth[1]; Michael Pütz[2]; Uwe Karst[1]; [1]*University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany;* [2]*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[1]; Kaytlin Krutsch[1]; Dhavalkumar Patel[1]; Teresa Baker[1]; [1]*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[1, 2]; Ismael Zamora[1]; Fabien Fontaine[1]; Albert Garriga[1]; Luca Morettoni[3]; Tatiana Radchenko[4]; [1]*Mass Analytica, S.L, Sant Cugat del Vallés, Spain;* [2]*Universitat Pompeu Fabra, Barcelona, Spain;* [3]*Mass Analytica, S.L, Bettona, Italy;* [4]*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[1]; Syeda Nazifa Wali[1]; Miranda Weigand[1]; Andrew Bowman[2]; David Wagner[2]; Julia Laskin[1]; [1]*Purdue University, West Lafayette, IN;* [2]*AbbVie Inc., North Chicago, IL*

MP 122 **Evaluation of potential spike-in proteins for normalization of TPP quantitation**; Chunna Guo[1]; Katelyn Caric[1]; Whitney Smith-Kinnaman[2]; Emma H Doud[2]; Amber L Mosley[2]; [1]*Indiana University, Indianapolis, IN;* [2]*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[1]; Liusheng Huang[2]; David Gingrich[1]; Francesca Aweeka[1]; [1]*University of California-San Francisco, San Francisco, CA;* [2]*University of California San Francisco, San Francisco, CA*

MP 124 **In vitroSR9011 metabolism study using tandem mass spectrometry**; Maxime Sansoucy[1]; Myriam Soucy[2]; Éric Morneau[1]; Benoit Daoust[2]; Simon Ricard[2]; Jean-François Naud[1]; [1]*Doping Control Laboratory - INRS, Laval, QC;* [2]*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-Hydroxyclarithromycin**; Xuguang Yan[1]; Zhijing Huang[1]; Moo-Young Kim[1]; Melissa Mofikoya[1]; [1]*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[1]; Claudia Boot[1]; *[1]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, Dolgoprudniy, Russian Federation*

MP 128 **Modelling ion trajectories in quadrupole fields using Python. A student exercise in our undergraduate chemical instrumentation course**; Robert L McClain[1]; John G Pavek[1]; John C. Wright[1]; *[1]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[1]; Tyler Hipple[1]; *[1]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[1]; Vladimir M. Doroshenko[1]; Nivedita Bhattacharya[2]; Madhuri Gupta[2]; Jan-Christoph Wolf[3]; Victor Laiko[1]; Enrico Davoli[4]; Venkat Panchagnula[1]; *[1]MassTech Inc., Columbia, MD; [2]Barefeet Analytics Pvt. Ltd., Pune, India; [3]Plasmion GmbH, Augsburg, Germany; [4]Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy*

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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[1]; Manorama Tummala[1]; *[1]Agilent Technologies, Singapore, Singapore*

MP 132 **Advancing Environmental Protection Through Real-Time Mobile, Fenceline, and Ambient Air Monitoring Solutions**; Paul Johnson[1]; Vaughan S. Langford[2]; Daniel B. Milligan[2]; Jihoon Lee[2]; Minyoung Cha[2]; *[1]Syft Techologies, Anaheim, CA; [2]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[1]; Benjamin Juba[1]; Yuliya Preger[1]; Reed Wittman[1]; Jill Langendorf[1]; Armando Fresquez[1]; Babu Chalamala[1]; *[1]Sandia National Laboratories, Albuquerque, NM*

MP 134 **Development of Novel Instrumentation Hyphenating Inductivly Coupled Plasma Mass Spectrometry with Colinear Resonance Ionisation Spectroscopy (ICP-MS-CRIS)**; Giles Edwards[1]; Matthew Duggan[1]; Holly Perrett[1]; Jordan Reilly[1]; Kieran Flanagan[1]; *[1]University of Manchester, Manchester, United Kingdom*

MP 135 **Unraveling Arsenic Speciation in Varied Food Matrices: Exploring Variability in High-Arsenic Foods**; Rachel R. Jones[1]; Kaitlyn Maloley[1]; Jacqueline Michelle Chaparro[1, 2]; Jessica E. Prenni[1]; *[1]Colorado State University, Fort Collins, CO; [2]Analytical Resources Core: Bioanalysis and Omics Center, Colorado State University, Fort Collins, CO*

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MP 136 **Characterization and evaluation of the environmental fate of aromatic hydrocarbons in weathered crude oil by using high-resolution orbitrap mass spectrometry**; Mark Romanczyk[1]; Christopher J Pfutzner[1]; *[1]Naval Research Laboratory, Washington, DC*

MP 137 **Online Chemical Analysis of Flowing Hydrocarbon Fuel Surrogates in a Pyrolysis Reactor by Molecular Beam Mass Spectrometry**; Andrew DeBlase[1, 2]; Matthew C Rohan[2]; Elizabeth S Kurian[2]; Alexander D Tucker[2]; Christopher R Bruening[1, 2]; William K Lewis[2]; *[1]University of Dayton Research Institute, Dayton, OH; [2]Air Force Research Laboratory, Aerospace Systems Directorate, Dayton, OH*

MP 138 **PETROLEUM AND ITS DISTILLATION CUTS ASSESSMENT: POLAR COMPOUNDS CHARACTERIZATION BY ORBITRAP HIGH RESOLUTION MASS SPECTROMETRY**; Thamara Barra[1]; Dayane Magalhães Coutinho[1]; Gutierri Ricardo dos Santos Gonçalves Salgueiro[1]; Alexandre de Oliveira Gomes[2]; Francisco Radler De Aquino Neto[1]; Débora de Almeida Azevedo[1]; *[1]UFRJ - Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [2]PETROBRAS, Rio de Janeiro, Brazil*

MP 139 **Complementarity of on-line RPLC x SFC-qTOF and SFC-FTICR for microalgae bio-oil characterization**; Jason Devaux[1, 2, 3]; Mélanie Mignot[1, 3]; Caroline Barrère-Mangote[3, 4]; Pierre Giusti[3, 4]; Sabine Heinisch[2]; Carlos Afonso[1, 3]; *[1]Laboratoire COBRA, Mont-Saint-Aignan Cedex, France; [2]Institut des Sciences Analytiques, Villeurbanne, France; [3]International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France; [4]TotalEnergies, Harfleur, France*

MP 140 **Characterization of re-refined base oils for lubricants using statistical approaches on Orbitrap mass spectrometry data**; Oscar Lacroix-Andrivet[1, 2, 3]; Marie Hubert-Roux[3, 4]; Anna Luiza Mendes Siqueira[2, 3]; Corinne Loutelier Bourhis[4]; Carlos Afonso[3, 4]; *[1]University of Rouen-Normandy, Mont-Saint-Aignan, France; [2]TotalEnergies OneTech, Centre de Recherche de Solaize (CRES), Chemin du canal, BP 22, 69360 Solaize, France, Solaize, France; [3]International Joint Laboratory—iC2MC: Complex Matrices Molecular Characterization, TRTG, BP 27, 76700 Harfleur, France, Harfleur, France; [4]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 141 **Brazilian crude oils compositional variations elucidated by pixel-based untargeted GC×GC–TOFMS data analysis**; Mônica Cardoso Santos[1]; Dayane Magalhães Coutinho[1]; Clarisse Lacerda Torres[1]; Manoel Mendes Alves Junior[1]; Michele Fabri de Resende[1]; Thamara Andrade Barra[1]; Vinícius Barreto Pereira[1]; Daniel Silva Dubois[2]; Joelma Pimentel Lopes[2]; Francisco Radler Aquino Neto[1]; Débora de Almeida Azevedo[1]; *[1]UFRJ - Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [2]PETROBRAS, Rio de Janeiro, Brazil*

MP 142 **Direct Analysis of Petroleum and Biofuels with FT-ICR MS and Direct Ionization Probe APPI**; Samuel P Putnam; *Bruker Scientific, Billerica, MA*

MP 143 **Biofuel extraction by ammonia from microalgal feed stock**; Takashi Ted Nohmi[1, 2]; Kiyoshi Sakuragi[3]; Toshio Mogi[2]; *[1]HysafeNohmi, Setagaya-Ku, Japan; [2]The university of Tokyo Department of Chemical System Engineering, Tokyo, Japan; [3]Central Research Institute of Electric Power Industry, Yokosuka, Japan*

MP 144 **Characterization of vacuum pump oils containing complex mixtures by combining multiple MS methods**; Kirk R Jensen[1]; Robert B Cody[1]; A John Dane[1]; *[1]JEOL USA, Inc., Peabody, MA*

MP 145 **Enhancing Petroleomics: Integrated Online SPE in FT-ICR MS for Complex Mixture Analysis – New solutions to Older Problems**; Nerilson MARQUES LIMA[1]; Hugo G Machado[2]; Gesiane da Silva Lima[2]; Joveilton Batista Da Silva Junior[2]; Gabriel Franco Dos Santos[2]; Andréa Rodrigues Chaves[2]; Alexandre A Ferreira[3]; Ygor S. Rocha[3]; Rodrigo Cabral da Silva[3]; Boniek Gontijo Vaz[2]; *[1]FEDERAL UNIVERSITY OF GOIAS, Goiânia, Brazil; [2]Federal University of Goias, Goiânia, Brazil; [3]PETROBRAS, Rio de Janeiro, Brazil*

MP 146 **Hidden Helpers: Metabolomic Analyses of Algae and Plants Reveal Dramatically Altered Metabolite Production in the Presence of Growth Promoting Bacteria**; Austin R Anderson[1, 2]; Sangeeta Negi[3]; Brett R. Blackwell[1, 2]; Kayla Kozisek[4]; Eric Robert Moore[3]; Abigale S

Mikolitis[1, 2]; Emilio S. Rivera[1, 2]; Chi-Yen Tseng[1, 2]; Ethan M. McBride[1, 2]; Phillip M. Mach[1, 2]; Zachary J. Sasiene[1, 2]; Grace M. Thornhill[1, 2]; Erick S. LeBrun[1, 2]; Joshua D. Breidenbach[1, 2]; Salvator J. Palmisano[1, 2]; Jessica A. Salguero[1, 2]; Francisca E. Rodriguez[1, 2]; Tara Harvey[1, 2]; Kes A. Luchini[1, 2]; Trevor G. Glaros[1, 2]; Lauren K. Heine[1, 2]; *[1]Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [2]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [3]Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [4]High Explosives Science and Technology Group, Weapon Stockpile Modernization Division, Los Alamos National Laboratory, Los Alamos, New Mexico*

MP 147 **Ageing effects of renewable synthetic and fossil fuels in a simulated technical environment**; Laurin Grabler[1]; Alessandro Vetere[1]; Wolfgang Schrader[1]; *[1]Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany*

MP 148 **Comparison of lignocellulosic-based biomass pyrolysis processes by multi-scale molecular characterization**; Charlotte MASE[1, 2]; Rémi Moulian[1, 2]; Eliane Lazzari[3]; Marco Piparo[1, 2]; Marie HUBERT-ROUX[2, 4]; Carlos AFONSO[2, 4]; David C. Dayton[5]; Caroline Barrère-Mangote[1, 2]; Pierre Giusti[1, 2]; *[1]TOTALENERGIES OT, Harfleur, France; [2]International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France; [3]Organic and Biological Analytical Chemistry Group, MolSys Research Unit, Liège, Belgium; [4]Univ Rouen Normandie, Rouen, France; [5]RTI International, Technology Advancement and Commercialization, Research Triangle Park, NC*

MP 149 **How can we gain structural information about individual compounds in complex mixtures: High resolution mass spectrometry meets theoretical calculations**; Wolfgang Schrader[1]; Jens Dreschmann[1]; Zahra Farmani[1]; Alessandro Vetere[1]; *[1]Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany*

MP 150 **Molecular characterization in Lithium-ion batteries: from electrolytes to electrodes**; Julien Maillard[1, 2]; Julien Demeaux[3]; Charlotte MASE[1, 2, 4]; Antonin Gajan[3]; Cécile Tessier[3]; Patrick Bernard[3]; Pierre Giusti[2, 4, 5]; Carlos Afonso[2, 4]; *[1]TOTALENERGIES OT, Harfleur, France; [2]International Joint Laboratory—iC2MC: Complex Matrices Molecular Characterization, TRTG, BP 27, 76700 Harfleur, France, Harfleur, France; [3]SAFT, Bordeaux, France; [4]University of Rouen-Normandy, Mont-Saint-Aignan, France; [5]TotalEnergies, Harfleur, France*

MP 151 **Utilizing a novel splitter to eliminate quantitation bias for simultaneous GCxGC-TOFMS/FID characterization of traditional and emerging fuels**; David E Alonso[1]; Joseph E Binkley[1]; John Hayes[1]; Elizabeth M Humston-Fulmer[1]; Christina N Kelly[1]; Dave Russ[1]; *[1]LECO Corporation, Saint Joseph, MI*

MP 152 **Optimization of Interfacial Material Isolation in Water-Oil Emulsions and Characterization by ESI(-)FT-ICR MS: A Centrifugation Method Approach**; Lindamara Maria de Souza[1, 2]; Eliane Valéria de Barros[3]; Luciara Costa De Souza[1]; Gabriely Silveira Folli[1]; Cristina Maria dos Santos Sad[1]; Danielle Mitze Muller Franco[4]; Gabriel Henry Morais Dufrayer[4]; Boniek Gontijo Vaz[4]; Marcio Nele de Souza[5]; Osvaldo Karnitz Jr[6]; Luiz Silvino Chinelatto Jr[6]; Marcia Cristina Khalil de Oliveira[6]; Valdemar Lacerda Jr[1]; Wanderson Romão[2, 7, 8]; *[1]Federal University of Espirito Santo, Vitória, Brazil; [2]National Institute of Forensic Science and Technology, INCT, Porto Alegre, Brazil; [3]Federal Institute of Education, Science and Technology of Espírito Santo, Vitória, Brazil; [4]Federal University of Goias, Goiania, Brazil; [5]Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [6]PETROBRAS, Rio de Janeiro, Brazil; [7]Federal Institute of Education, Science and Technology of Espírito Santo, Vila Velha, Brazil; [8]Federal University of Espírito Santo, Vitória, Brazil*

MP 153 **ESI(-)FT-ICR MS applied in the study of interfacial materials of Brazilian crude oils**; Eliane Valéria de Barros[1]; Lindamara Maria de Souza[2]; Luciara Costa De Souza[3]; Cristina Maria dos Santos Sad[3]; Danielle Mitze Muller Franco[4]; Gabriel Henry Morais Dufrayer[4]; Boniek Gontijo Vaz[4]; Márcio Nele de Souza[5]; Osvaldo Karnitz Jr[6]; Luiz Silvino Chinelatto Jr[6]; Marcia Cristina Khalil de Oliveira[6]; Valdemar Lacerda Jr. [3]; Wanderson Romão[3, 7]; *[1]Federal Institute of Education, Science and Technology of Espírito Santo, Vitória, Brazil; [2]Federal University of Espírito Santo, Vitória, Brazil; [3]Federal University of Espirito Santo, Vitória, Brazil; [4]Federal University of Goias, Goiania, Brazil; [5]Federal University of Rio de Janeiro, Rio de Janeiro, Brazil; [6]PETROBRAS, Rio de Janeiro, Brazil; [7]Federal Institute of Education, Science and Technology of Espírito Santo, Vila Velha, Brazil*

MP 154 **Direct APCI: A Straightforward Method for Precision Analysis of Sulfur-Containing Compounds in Complex Mixtures**; Danielle Mitze[1]; Taynara Covas[1]; Rosana Cardoso[1]; Lidya Cardozo[1]; Mário Rangel[1]; Rosineide Simas[2]; Gabriel Henry Dufrayer[1]; Boniek Gontijo[1]; *[1]Federal University of Goias, Goiania, Brazil; [2]Mackenzie University, São Paulo, Brazil*

MP 155 **Finding needles in haystacks: Using statistical tools for complex samples measured by using GCxGC-HRMS**; John Dane[1]; Scott J. Campbell[2]; John Moncur[2]; Kirk R Jensen[1]; Robert B Cody[1]; *[1]JEOL USA, Inc., Peabody, MA; [2]SpectralWorks Ltd, Runcorn, United Kingdom*

MP 156 **Influence of Metals On Asphaltenes' ESR, Ion Mobility, Mass, and NMR Spectra: An Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) Study**; Sahil Makhani[1]; Thanuja M Thilakarathna[1]; Bismark Nyaabak[1]; Patrick J. Farmer[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

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MP 157 **Measurement of Medium and Long Chlorinated Alkanes in Canadian Biota and Analysis by LC Orbitrap**; Helena Steer[1]; Beau Atkinson[1]; Adnan Chowdhury[1, 2]; *[1]Environment Canada, Burlington, ON; [2]Western University, London, ON*

MP 158 **A Penguin's Perspective: Silicone wristbands as passive samplers to explore exposure of Megellanic Penguins to emerging and leacy contaminants**; Paige Montgomery[1]; Jonathan Navarro-Ramos[1]; Ralph Eric Thijl Vanstreels[2]; Logan Running[1]; Katarzyna Kordas[3]; Diana S Aga[1, 4]; *[1]Department of Chemistry, The State University of New York at Buffalo, Buffalo, NY; [2]University of São Paulo. Department of Pathology. Laboratory of Comparative Pathology of Wild Animals, Butantã, Brazil; [3]Department of Epidemiology and Environmental Health, The State University of New York at Buffalo, Buffalo, NY; [4]RENEW Institute, The State University of New York at Buffalo, Buffalo, NY*

MP 159 **Non-target Identification of Harmful Organic Compounds in Weathered Marine Microplastics by High-Resolution Gas Chromatography-Time-of-Flight-Mass Spectrometry**; Patrick T Justen[1]; Emily Böckenholt[2]; Susan D Richardson[1]; Mohammed Baalousha[1]; *[1]University of South Carolina, Columbia, SC; [2]University of Duisburg Essen, Duisburg, Germany*

MP 160 **Characterizing novel, sorbent-based pre-concentration methods for trace detection of perfluoroalkyl substances with ambient pressure mass spectrometry**; Nathan Robert Bays[1]; David Shafer[1]; Andre Benally[1]; Mohammad Shohel[1]; Troy Bencoe[1]; Mark Rigali[1]; Jessica Kustas[1]; Andrew W. Knight[1]; Ryan D. Davis[1]; *[1]Sandia National Lab, Albuquerque, NM*

MP 161 **Innovation Development of Multidimensional Holographic Analysis Technology of the Pre- and Polyfluoroalkyl Substances in Environmental Water**; Shan-An Chan[1]; Yue Song[2]; Hui XU[2]; *[1]Agilent Technology,* *Inc., Taipei, Taiwan; [2]Agilent Technology, Inc., Shanghai, China*

MP 162 **Utilizing cost effective helium saving technology for low level quantitationof Polychlorinated dibenzo-p-dioxins/furans using gas chromatograph mass spectrometry**; Adam Ladak[1]; Paul Silcock[1]; Nicholas Warner[2]; Daniel Kutscher[2]; Amit Gujar[3]; Jason Cole[3]; Xin Zheng[3]; *[1]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermo Fisher Scientific, Bannockburn, IL*

MP 163 **Paper Spray High-Resolution Tandem Mass Spectrometry (PS-HRMS/MS) for Rapid, Multi-class Cyanotoxin Analysis**; Lucas R. Abruzzi[1, 2]; Daniel G. Beach[3]; Erik T Krogh[1, 2]; Christopher G. Gill[1, 2, 4, 5, 6]; *[1]Appl. Env. Res. Labs. (AERL), Nanaimo, BC; [2]University of Victoria, Victoria, BC; [3]National Research Council Canada, Halifax, NS; [4]Vancouver Island University, Nanaimo, BC; [5]Simon Fraser University, Burnaby, BC; [6]University of Washingon, Seattle, WA*

MP 164 **Rapid and highly sensitive quantitation of Microcystins and Nodularin in water by modern LC-MS/MS**; Kate (Xiaomeng) Xia[1]; Evelyn Wang[1]; Ruth Marfil-Vega[1]; Yoshiyuki Okamura[1]; Tairo Ogura[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

MP 165 **Pyrolysis gas chromatography-cyclic ion mobility mass spectrometry reveals micro-/nanoplastics in placental tissue of Canadians**; Nikita E. Harvey[1]; Justine R. Bissonnette[1]; Darcie Stapleton[1]; Catherine M.E. Barrett[1]; Lindsay S. Cahill[1]; Karl J. Jobst[1]; *[1]Memorial University of Newfoundland, St. John's, NL*

MP 166 **Characterization of microplastics in the maternal blood of Canadians by pyrolysis gas chromatography-cyclic ion mobility mass spectrometry**; Justine R. Bissonnette[1]; Nikita E. Harvey[1]; Lindsay S. Cahill[1]; Karl J. Jobst[1]; *[1]Memorial University of Newfoundland, St. John's, NL*

MP 167 **Per- and Polyfluoroalkyl Substances in Aqueous Samples: Performance Demonstration of EPA Method 1633 Using High Sensitivity Mass Spectrometry**; Megan P Davis[1]; Om K Shrestha[1]; Kathleen K Luo[1]; Landon A Wiest[1]; Evelyn H Wang[1]; Michelle Zipse[1]; Keith Herman[1]; *[1]SSI, Columbia, MD*

MP 168 **Intensive temporal sampling for the emerging salmon toxin 6PPD quinone by condensed phase membrane introduction mass spectrometry**; Angelina Jaeger[1, 2]; Joseph Monaghan[1]; Haley Tomlin[3]; Jamieson Atkinson[3]; Chris G Gill[1, 2, 4, 5]; Erik T Krogh[1, 2]; *[1]Vancouver Island University, Nanaimo, BC; [2]University of Victoria, Victoria, BC; [3]British Columbia Conservation Foundation, Nanaimo, BC; [4]Simon Fraser University, Burnaby, BC; [5]University of Washington, Seattle, WA*

MP 169 **Crowdsourcing Citizens for Statewide Mapping of PFAS in Florida Drinking Water**; Thomas Sinkway; *University of Florida, Gainesville, FL*

MP 170 **Evaluation of Extremophile Methylorubrum extorquens for Treatment of Oilsands-Derived Naphthenic Acid Fraction Compounds by Orbitrap Mass Spectrometry**; Ian J Vander Meulen[1, 2]; Jordyn Bergsveinson[2]; Dena W McMartin[1, 3]; John Headley[2]; *[1]University of Saskatchewan, Saskatoon, SK; [2]Environment Canada, Saskatoon, SK; [3]University of Lethbridge, Lethbridge, AB*

MP 171 **A high-throughput analysis workflow to characterize Pharmaceuticals and personal care products (PPCPs) in aquatic environment**; SHENGLAN JIA[1]; Mauricius Marques Dos Santos[1]; Shane Allen Snyder[1]; *[1]Nanyang Technological University, NEWRI, Singapore, Singapore*

MP 172 **Expanding the chemical space of the fragmentation spectra-based exposure prediction model**; Helen Sepman[1, 2]; Drew Szabo[1]; Gordian Sandberg[1]; Ida Rahu[1]; Irene Pulido Campillo[1]; Emma Apelgren[1]; Anneli Kruve[1, 2]; *[1]Department of Materials and Environmental Chemistry, Stockholm University, Stockholm, Sweden; [2]Department of Environmental Science, Stockholm University, Stockholm, Sweden*

MP 173 **Disinfection By-products from Water Chlorination Reconfirmed by Electrochemistry-MS**; Jean-Pierre Chervet[1]; Albert T LEBEDEV[2]; Martin Eysberg[3]; Hendrik-Jan Brouwer[4]; *[1]Antec Scientific, Alphen a/d Rijn, Netherlands; [2]Department of Materials Science, MSU-BIT University, Shenzhen 517182, China; [3]Antec Scientific, Boston, MA; [4]Antec Scientific, Alphen aan den Rijn, Netherlands*

MP 174 **A novel approach for monitoring multi-classes of POPs in a single run by GC-Ion Mobility-HRMS**; Arnd Ingendoh[1]; Carsten Baessmann[1]; Javier Lopez[1]; Miguel Angel Perez[1]; Hugo Muller[2]; Gauthier Eppe[3]; *[1]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; [2]Mass Spectrometry Laboratory, MolSys Research Unit, Chemistry Department, University of Liège, Liege, Belgium; [3]Mass Spectrometry Laboratory, MolSys Research Unit, University of Liege, Liege, Belgium*

MP 175 **Sewage Proteomics: What can we learn?**; Ester Sánchez-Jiménez[1, 2]; Carlos Pérez-López[2]; Antonio Ginebreda[2]; Joaquin Abian[1]; Damià Barceló[2]; Montserrat Carrascal[1]; *[1]Biological and Environmental Proteomics, Institute of Biomedical Research of Barcelona, Spanish National Research Council (IIBB-CSIC/), Barcelona, Spain; [2]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 176 **Optimized gas chromatography-electron impact ionization-tandem mass spectrometry for simultaneous quantification of 12 novel brominated flame retardants in agricultural products**; Juyoun Lee[1]; Minki Shim[1]; Hyojeong Lee[1]; Dong-Kyu Lee[1]; *[1]College of Pharmacy, Chung-Ang University, Seoul, South Korea*

MP 177 **Determination of Glyphosate, Aminomethylphosponic Acid (AMPA), and Glufosinate in Drinking Water Using Direct Analysis by LC-MS/MS**; Narendra Meruva[1]; Stuart J Adams[2]; Benjamin Wuyts[3]; Simon Hird[2]; *[1]Waters Corporation, Milford, Massachusetts; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters Corporation, Antwerp, Belgium*

MP 178 **Expanding a High-Quality Environmental Reference Electron Ionization Mass Spectral Library**; Yufang Zheng[1]; Edward P. Erisman[1]; Weihua Ji[1]; Tytus Mak[1]; Quan-Long Pu[1]; Stephen E Stein[1]; William E Wallace[1]; *[1]NIST, Gaithersburg, MD*

MP 179 **Harnessing the Power of Mass Spectrometry and Automation to Reduce Sample Size, Sample Preparation Time and Increase Laboratory Efficiency**; Kari Organtini[1]; Chelsea Plummer[1]; Kenneth Rosnack[1]; Oliver Burt[2]; Ian Wan[3]; *[1]Waters Corporation, Milford, Massachusetts; [2]Waters Corporation, Wilmslow, United Kingdom; [3]PromoChrom Technologies, Richmond, BC*

MP 180 **Analysis of High Mass Polycyclic Aromatic Hydrocarbons (PAHs) Extracted from Microplastics Spilled in the Marine Environment**; Douglas Stevens[1]; Christopher Reddy[2]; Bryan James[2]; Robert Nelson[2]; Frank L. Dorman[1]; Sarah Dowd[1]; *[1]Waters Corporation, Milford, Massachusetts; [2]Woods Hole Oceanographic Institution, Falmouth, MA*

MP 181 **Suspect and non-targeted screening of halogenated contaminants in a stranded killer whale (Orcinus orca) using GC-HRMS hyphenated with TIMS**; Hugo Muller[1]; Krishna Das[2]; George Scholl[1]; Emma L. Schymanski[3]; Gauthier Eppe[1]; *[1]Mass Spectrometry Laboratory, MolSys Research Unit, University of Liege, Liege, Belgium; [2]Freshwater and Oceanic ScienCes Unit of ReSearch (FOCUS), Laboratory of Oceanology, University of Liège, Liège, Belgium; [3]Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Luxembourg, Luxembourg*

MP 182 **Quantification of Microplastics and Nanoplastics in biosolids**; Tommy M Nguyen[1]; O. David Sparkman[2]; Liang Xue[2]; Harry Allen[3]; Terry Ramus[4]; Ichi Watanabe[5]; *[1]University of The Pacific, Stockton, CA; [2]University of the Pacific, Stockton, CA; [3]U.S. Environmental Protection Agency, Arcadia, CA; [4]Diablo Analytical, Antioch, CA; [5]Frontier Laboratories, Koriyama, Japan*

MP 183 **Statewide surveillance and mapping of PFAS in Florida surface water**; Camden Camacho[1]; John Bowden[1]; *[1]University of Florida, Chemistry Department, Analytical Chemistry Division, Gainesville, FL*

MP 184 **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[1]; Joe Binkley[2]; *[1]Leco Corporation, St. Joseph, MI; [2]LECO Corporation, Saint Joseph, MI*

MP 185 **Residential exposure to micro-/nanoplastics in indoor air studied by pyrolysis gas chromatography-cyclic ion mobility mass spectrometry**; Mikela L Rowsell[1]; Frank L. Dorman[2]; Lindsay S. Cahill[3]; Karl J Jobst[3]; *[1]Memorial University of Newfoundland, St.John's, NL; [2]Waters Corporation, Milford, Massachusetts; [3]Memorial University of Newfoundland, St. John's, NL*

MP 186 **Characterization of hydrothermal liquefaction products of kraft lignin using high-resolution ESI/APPI FT-ICR MS**; Mahmoud Negm[1]; Eemeli Eronen[1]; Mikko Nikunen[1]; Janne Jänis[1]; *[1]University of Eastern Finland, Joensuu, Finland*

MP 187 **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[1]; Michal Marszewski[1]; Dragan Isailovic[1]; *[1]University of Toledo, Toledo, OH*

MP 188 **Identification of Novel Cyanopeptolins in Lake Erie CyanoHAB Samples using UHPLC-HRMS and HRMS/MS**; Sharmila I Thenuwara[1]; Judy A Westrick[2]; Dragan Isailovic[1]; *[1]University of Toledo, Toledo, OH; [2]Wayne State University, Detroit , MI*

MP 189 **Identification of Degradation Products of Cellulose Derivatives in Soil**; Cole D. Babcock[1, 2]; Ayden S Justice-Riar[1]; Seth Nobert[1]; Emmanuel Mapfumo[1]; Makan Golizeh[1]; *[1]Concordia University of Edmonton, Edmonton, AB; [2]Babcocks Synthetics Ltd., Wainwright, AB*

MP 190 **Rapid Degradation of Per- and Polyfluoroalkyl Substances (PFAS) in Microdroplets**; Md. Tanim-Al Hassan[1]; Yongqing Yang[1]; Richard N Zare[2]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]Stanford University, Stanford, CA*

MP 191 **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 192 **Soot-on-snow: Comprehensive chemical fingerprinting of combustion-derived organic aerosols deposited on snow using APPI/ESI FT-ICR mass spectrometry**; Timo Kekäläinen[1]; Mikko Nikunen[1]; Hans Moosmüller[2]; Jonas Svensson[3]; Krista Luoma[3]; Delun Li[3]; Outi Meinander[3]; Anna Kontu[4]; Oona Norvapalo[5]; Pavla Dagsson-Waldhauserova[6]; Aki Virkkula[3]; Olli Sippula[5]; Janne Jänis[1]; Jie Guo[1]; Niko Kinnunen[1]; *[1]University of Eastern Finland, Joensuu, Finland; [2]Division of Atmospheric Sciences, Desert Research Institute (DRI), Reno, NV; [3]Atmospheric Composition Unit, Finnish Meteorological Institute, Helsinki, Finland; [4]Earth Observation Research, Finnish Meteorological Institute, Sodankyla, Finland; [5]Department of Environmental and Biological Sciences, University of Eastern Finland, Kuopio, Finland; [6]Faculty of Environmental and Forest Sciences, Agricultural University of Iceland, Reykjavik, Iceland*

MP 193 **Method Development and Validation for Trace Determination of Aryl and Alkyl Organophosphate Esters in Surface Waters by LC-MSMS**; Beau W Atkinson[1]; JoAnne Schachtschneider[1]; *[1]Environment Canada, Burlington, ON*

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MP 194 **Determination of emerging contaminants in ambient water using an ultra-sensitive triple quadrupole mass spectrometer**; Guangning Li[1]; Xiaojie Sun[2]; Bingjie Liu[2]; Lihai Guo[2]; *[1]SCIEX, Beijing, China; [2]SCIEX, Beijing, China*

MP 195 **Evaluation of Dielectric Barrier Discharge Ionization (DBDI) for the Identification of Xenobiotic Environmental Metabolites and Degradation Products**; Jeffrey R Gilbert[1]; David K Robbins[1]; Chris Brown[1]; Krishna Kuppannan[1]; David Hills[1]; Chengli Zu[1]; *[1]Corteva Agriscience, Indianapolis, IN*

MP 196 **LC-MS/MS assay for Quantitative Analysis of Long Acting Anti Coagulants (LAARs) in Plasma and Extracellular Vesicles from Rabbits**; Intakhar Ahmad[1]; Ruth N Muchiri[2]; Richard B van Breemen[2]; Douglas Feinstein[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]Oregon State University, Corvallis, OR*

MP 197 **Assessing Antidepressant Pharmaceuticals in the Environment through the Development of a Multidimensional Liquid Chromatography-Ion Mobility Spectrometry-Mass Spectrometry Library**; Emily K Crawford[1]; James N. Dodds[1]; Erin S. Baker[1]; *[1]UNC-Chapel Hill, Chapel Hill, NC*

MP 198 **Characterization of organic and inorganic analytes in snow made from reclaimed water at Arizona Snowbowl Ski Resort**; Marquis T. Yazzie[1]; Haoqi Nina Zhao[2]; Anita J. Antoninka[3]; Pieter C. Dorrestein[2]; Catherine R. Propper[3]; Jani C. Ingram[3]; Allegra T. Aron[1]; *[1]University of Denver, Denver, CO; [2]University of California San Diego, La Jolla, CA; [3]Northern Arizona University, Flagstaff, AZ*

MP 199 **Format Comparison for Dispersive Solid Phase Extraction (dSPE) Workflow Improvements for Food Testing Prior to GC/MS Analysis**; Lucy Lund[1]; Russell Parry[1]; Lee Williams[1]; Geoff Davies[1]; Alan Edgington[1]; Adam Senior[1]; Helen Lodder[1]; Zainab Khan[1]; Claire Desbrow[1]; Dan Menasco[1]; *[1]Biotage GB Limited, Cardiff, United Kingdom*

MP 200 **Comprehensive pesticide screening by column-switching LC-MS/MS using multiple activation methods CID, EAD and UVPD**; Romain GIRAUD[1]; Mircea Guna[2]; Yves LeBlanc[2]; Gérard Hopfgartner[1]; *[1]LSMS, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; [2]SCIEX, Concord, ON*

MP 201 **Making Crayfish Happy: Using LC-MS/MS to Evaluate the Nervous System of Procambarus clarkii Following Exposure to SSRIs and SNRIs**; Claire Korte[1]; Sydney Worth[1]; Jillian Tonnies[1]; Corina Trapp[1]; Muskan Bakshi[1]; Kevin Tucker[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL*

MP 202 **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 Arigò[1]; Giovanna Nevola[1]; Giorgio Famiglini[1]; Pierangela Palma[1, 2]; Achille Cappiello[1, 2]; *[1]University of Urbino Carlo Bo, Urbino, Italy; [2]Vancouver Island University, Nanaimo, BC*

MP 203 **MALDI MSI Matrix Optimization for the Analysis of Lipid-Related Metabolites in Earthworms Exposed to Statins as Environmental Contaminants**; Kendra G. Selby[1]; Lauren H. Phan[1]; Claire E. Korte[1]; Gabriel A. Bressendorff[1]; M Nazim Boutaghou[2]; Kevin R. Tucker[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL; [2]Shimadzu Scientific Instruments, Columbia, MD*

MP 204 **Identification of anthropogenic compounds in stream waters using non-target strategies by HRMS**; Imma Ferrer[1]; Michael Thurman[1]; James S Pyke[2]; Andrew McEachran[2]; *[1]University of Colorado, Boulder, CO; [2]Agilent Technologies, Santa Clara, CA*

MP 205 **Non-Target HRMS: Quantifying Emerging Contaminants in Saudi Arabian Water, Soil, and Plants under Extreme**

Climate (40-45°C); Damia Barcelo[1]; Yolanda Pico[2]; Julian Campo[2]; Mohamed El-Sheik[3]; Ahmed H Alfarhan[3]; *[1]IDAEA-CSIC, Barcelona, Spain; [2]SAMA-UV, Moncada, Spain; [3]King Saud University, Riyadh, Saudi Arabia*

MP 206 **Ultra-Sensitive Dynamic Headspace GC-MS/MS method for trace level quantitation of Nitrosamines in Deferiprone API**; Durvesh Sawant[1]; Hemant Kesarkar[1]; Sanket Chiplunkar[1]; Prashant Hase[1]; Aseem Wagle[1]; Rahul Dwivedi[1]; Siddhata Jadhav[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; Satyendra Singh[1]; Mohit Sharma[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

MP 207 **Simultaneous determination of known and unknown Extractables in pharmaceuticals packaging material by tandem mass spectrometry using Scan-MRM mode**; Hemant Kesarkar[1]; Sanket Chiplunkar[1]; Prashant Hase[1]; Durvesh Sawant[1]; Aseem Rajan Wagle[1]; Rahul Dwivedi[1]; Siddhata Jadhav[1]; Satyendra Singh[1]; Mohit Sharma[1]; Pratap Rasam[1]; Jitendra Kelkar[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

EXTRACTABLES & LEACHABLES
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MP 208 **Enhanced Detection Sensitivity of Volatile Extractables in Aqueous Extracts through Dynamic Headspace GC-MS Analysis**; Samanthi I Wickramasekara[1]; Milani Wijeweera Patabandige[1]; Amali Herath[1]; Jacob Hill[1]; *[1]U.S. Food and Drug Administration, Silver Spring, MD*

MP 209 **GC/MS approach for analysis of extractables and leachables (E&L) in complex matrices using spectral deconvolution and retention indices**; Bruce Quimby[1]; Anastasia Andrianova[1]; Sofia Nieto[2]; Lakshmi Krishnan[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Santa Clara, CA*

MP 210 **Combined qualitative and quantitative analysis of food packaging materials using QTOF mass spectrometry**; Jack Steed[1]; Jianru Stahl-Zeng[2]; Daqiang Pan[2]; Clemens Bidmon[3]; *[1]SCIEX, Macclesfield, United Kingdom; [2]SCIEX, Darmstadt, Germany; [3]TÜV Rheinland, Nuremberg, Germany*

MP 211 **Combined LC/MS and GC/MS approach for analysis of extractables and leachables in complex matrices using high resolution mass spectrometry**; Sofia Nieto[1]; David Weil[1]; Matthew Curtis[1]; Lee Bertram[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

MP 212 **Effects of Extraction Conditions and Sample Preparation on Extractables from Medical Devices by LC-UV/MS**; JoAnn C Chen[1]; Peifeng Hu[1]; D. Paul Cole[1]; *[1]Baxter Healthcare Corporation, Round Lake, IL*

MP 213 **Identification and Profiling of an Unknown in Base E-Liquid Formulations**; Diane Wallace[1]; Aliya Al-Habsha[1]; Matthew Lyndon[1]; Xin Yang[1]; Karen Carter[1]; Norman Fraley[1]; I. Gene Gillman[1]; *[1]Juul Labs, Washington, DC*

MP 214 **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[1]; Eric Hill[2]; *[1]LECO Corporation, St. Joseph, MI; [2]Boston Analytical, Salem, NH*

MP 215 **Headspace-SIFT-MS: Rapid Screening of Hazardous Volatile Impurities in Haircare and Skincare Products**; Luke Thomason[1]; Mark J. Perkins[2]; Colin J. Hastie[2]; Vaughan S. Langford[1]; Leslie P. Silva[3]; *[1]Syft Technologies, Christchurch, New Zealand; [2]Element Lab Solutions, Cambridge, United Kingdom; [3]Syft Technologies, Los Angeles, CA*

MP 216 **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[1]; Becky Bader[1]; Norma Turner[1]; *[1]Cambridge Polymer Group, Woburn, MA*

MP 217 **Non-targeted analysis, interactive visualization, and online sharing of interactive LC-HRMS/MS data of polymers using a comprehensive software PolyMatch Suite**; Jeremy Koelmel[1]; David A Weil[2]; Emma E. Rennie[2]; Paul Stelben[1]; Nicholas Oranzi[3]; Michael Kummer[4]; David Godri[5]; Jiarong Qi[1]; Elizabeth Z. Lin[1]; Krystal J. Godri Pollitt[1]; *[1]Yale University, New Haven, CT; [2]Agilent Technologies, Santa Clara, CA; [3]University of Florida, Gainesville, FL; [4]Innovative Omics, Sarasota, FL; [5]3rd Floor Solutions, Caledon, Ontario*

MP 218 **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[1]; Lee Bertram[1]; Sierra D. Durham[1]; Olivier Chevallier[1]; Kai Chen[1]; *[1]Agilent Technologies, Santa Clara, CA*

FOOD SAFETY & CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS, AND SUPPLEMENTS
219-237

MP 219 **High-sensitivity, high-throughput pesticide analysis by micro-flow LC-MS**; Runsheng Zheng[1]; Christopher Pynn[1]; Stephanie Koczur[1]; Katherine Lovejoy[1]; Ece Aydin[1]; Alec Valenta[1]; Kenneth Matuszak[2]; Wim Decrop[1]; Martin Samonig[1]; *[1]Thermo Fisher Scientific, Germering, Germany; [2]Thermo Fisher Scientific, West Palm Beach, FL*

MP 220 **Metabolomic and Proteomic Analysis Reveals Compositional Differences in Beer Clarified Using Ultrasonic Filtration as Compared to Centrifugation**; Brett R Blackwell[1]; James E Coons[2]; Chi-Yen Tseng[1]; Kes A. Luchini[1]; Bert Boyce[3]; Jeff Erway[4]; Joel Gregory[5]; Rich Headley[6]; Phillip M. Mach[1]; Trevor G. Glaros[1]; *[1]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [2]Los Alamos National Laboratory, Los Alamos, NM; [3]Santa Fe Brewing Company, Santa Fe, NM; [4]La Cumbre Crewing Company, Albuquerque, NM; [5]Ex Novo Brewing Company, Corrales, NM; [6]Beer Creek Brewing Company, Santa Fe, NM*

MP 221 **Identification of Double-Bond Position in Cyclic Ester using OAD-TOF system**; Yohei Arao[1]; Jun Kurabe[2]; Hidenori Takahashi[1]; Akihiro Kawaraya[2]; *[1]Shimadzu Corporation, Nakagyo-ku, Japan; [2]TAKASAGO INTERNATIONAL CORPORATION, Hiratsuka, Japan*

MP 222 **Characterization of Dietary Xylans and Arabinoxylans by LC-MS: Implications for Enhancement of Prebiotic Activity with Supplemental Enzymes In Situ**; James G Farmar[1]; Caroline H. Best[1]; Kelly M. Tinker[1]; Sean M. Garvey[1]; *[1]BIO-CAT, Troy, VA*

MP 223 **Non-targeted analysis of mushroom-containing coffee products using ion mobility-high resolution mass spectrometry**; Lindsay E Hatch[1]; Gordon T Fujimoto[1]; Emily R Britton[1]; *[1]Waters Corporation, Milford, MA*

MP 224 **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[1]; Zhenghua Rao[2]; Yaxiong Jia[3]; *[1]Institute of Animal Sciences, CAAS, Beijing, China; [2]Institute of Animal Sciences of Chinese Academy of Agricultural Sciences, BEIJING, China; [3]Institute of Animal Sciences, Chinese Academy of Agricultural Sciences, BEIJING, China*

MP 225 **Discovery of Synthetic Cooling Agents in Consumer Products using a Standardized Screening Approach**; Benjamin Katz; *UC Irvine, Irvine*

MP 226 **Comprehensive Metabolomic Profiling of Coffea canephora Coffees during roasting stages by ESI(±)LTQ MS**; Eustaquio V. R. De Castro[1, 2]; Danieli G. Debona[1]; Marcos Valério V. Lyrio[1, 3]; Lucas L. Pereira[4]; Amanda E. Feu[3]; Emanuele C. S. Oliveira[4]; Roberta Q. Frinhani[1]; Wanderson Romao[3, 5]; *[1]Coffee Chemistry Laboratory - Coffee Design Group, Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil; [2]Laboratory for Research and Development of Methodologies for Oil Analysis / LabPetro, Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil; [3]Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espirito Santo, Vitória, Brazil; [4]Coffee Design. Federal Institute of Espírito Santo, Venda Nova do*

Imigrante, Brazil; [5]Federal Institute of Espírito Santo, Brazil, Vitoria, Brazil

MP 227 **Absolute Quantification of Polysaccharides in Mushrooms using LC-MS/MS Platform**; Sophia Jiang[1]; Shawn Ehlers-Cheang[2]; Christopher Suarez[2]; Katherine Phillips[3]; Naomi Fukagawa[4]; Carlito B. Lebrilla[2]; *[1]University of California, Davis, Davis, CA; [2]University of California Davis, Davis, CA; [3]Virginia Tech, Blacksburg, Virginia; [4]Beltsville Human Nutrition Research Center, Beltsville, Maryland*

MP 228 **Royal jelly's phenolic profile via UPLC-VIP-HESI-TIMS-QTOF-MS: A thorough characterization following a multivariate optimization approach**; Elena S. Nastou[1]; Dafni V. Preza-Mayo-Kataki[1]; Panagiotis- Loukas P. Gialouris[1]; Carsten Baessmann[2]; Nikolaos S. Thomaidis[1]; *[1]National and Kapodistrian University of Athens, Department of Chemistry, Laboratory of Analytical Chemistry, Athens, Greece; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

MP 229 **Development of a Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) Targeted Screening Method for Food Additives**; Jessica K Beekman[1]; Katherine Carlos[1]; *[1]U.S. Food and Drug Administration, Center for Food Safety and Applied Nutrition, 5001 Campus Drive, College Park, MD*

MP 230 **Give it Your All or Just 80%?: The Impact of Resuspension Solvent Composition for Standardized Nontargeted Metabolomics Analysis of Food**; Margaret Read[1]; Melanie T Odenkirk[1]; Jacqueline Michelle Chaparro[1]; Sahar B Toulabi[1]; Corey D Broeckling[1]; Cole Michel[2]; Arpana Vaniya[3]; Katrina Doenges[2]; Sarah Brinkley[4]; Katrina L Leaptrot[5]; Stacy D Sherrod[5]; Jody C May[5]; Nathan Montgomery[1]; Richard Reisdorph[2]; Nichole Reisdorph[2]; John A McLean[5]; Oliver Fiehn[3]; Chi-Ming Chen[6]; Tracy Shafizadeh[6]; Steve Watkins[6]; Jessica E Prenni[1]; *[1]Colorado State University, Fort Collins, CO; [2]University of Colorado, Anschutz Medical Campus, Department of Pharmaceutical Sciences, Aurora, CO; [3]University of California Davis, Davis, CA; [4]The Alliance of Bioversity International & The International Center for Tropical Agriculture (CIAT), Cali, Colombia; [5]Vanderbilt University, Nashville, TN; [6]Verso Biosciences, Davis, CA*

MP 231 **Direct Analysis in Real-Time with High Resolution Mass Spectrometry: A Rapid Tool for Black Truffle Authentication**; Ilona Nordhorn[1]; Klemens Losso[2]; Matthias Rainer[3]; John (Jay) Brann[4]; Carsten Baessmann[1]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]MCI | The Entrepreneurial School, Innsbruck, Austria; [3]Leopold-Franzens University of Innsbruck, Innsbruck, Austria; [4]Bruker Daltonics GmbH & Co. KG, Billerica, MA*

MP 232 **Fabric Phase Sorptive Extraction method for the determination of veterinary drugs, pesticides and mycotoxin in milk by LC-HRMS**; Belete E Gebreyohannes[1]; Simiso Dube[1]; Mathew MM Nindi[1]; *[1]University of South Africa, , Florida Park, Roodepoort, South Africa*

MP 233 **Quantification of Hop-Derived Bitter Compounds in Beer Using Liquid Chromatography Mass Spectrometr**; Chieh-En Teng[1]; Yumeng Wang[1]; Tai-Huan Li[2]; Sung-Fang Chen[1]; *[1]National Taiwan Normal University, Taipei, Taiwan; [2]Zhangmen Brewing Company, New Taipei City, Taiwan*

MP 234 **Simultaneous analysis of organophosphate flame retardants in food samples by LC-MS/MS**; Taek Gu Han[1]; Eun Seon Jeong[1]; Jong Seong Kang[1]; Hyung Min Kim[1]; *[1]College of Pharmacy, chungnam University, Daejeon, South Korea*

MP 235 **Quantitation of alpha lactalbumin and beta lactoglobulin in infant formula and milk products**; Jeff Shippar; *Eurofins, Madison, WI*

MP 236 **Application of untargeted headspace solid-phase microextraction-gas chromatography-mass spectrometry for volatile metabolomics-based authentication of plant-based milk alternatives**; Tianqi Li[1]; Renato Handoyo[1]; Enea Pagliano[2]; Yaxi Hu[3]; *[1]Carleton University, Ottawa, ON; [2]National Research Council of Canada, Ottawa, ON; [3]Carleton University, Department of Chemistry, Ottawa, ON*

MP 237 **Identifying Allergen ELISA Target Proteins using Mass Spectrometry**; Ellenor R Sell[1]; Justin T Marsh[2]; Joseph L Baumert[2]; Philip E Johnson[2]; *[1]University of Nebraska - Lincoln, Lincoln, NE; [2]Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, Nebraska, Lincoln, NE*

FUNDAMENTALS: ION ACTIVATION/DISSOCIATION
238-248

MP 238 **Intact Transition Epitope Mapping – Force Interferences by Variable Extensions (ITEM-FIVE)**; Cornelia Koy[1]; Claudia Röwer[2]; Andrei Neamtu[3]; Hans-Jürgen Thiesen[4]; Michael O. Glocker[2]; *[1]Proteome Center Rostock, Rostock, Germany; [2]Proteome Center Rostock, Rostock, Germany; [3]TRANSCEND Centre – Regional Institute of Oncology (IRO), Iasi, Romania; [4]Institute of Immunology, Rostock, Germany*

MP 239 **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[1]; Axe Xie[1]; Emily Zahn[1]; Zongtao Lin[1]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, Saint Louis, MO*

MP 240 **Photoactivated radical induced dissociation is sensitive to gas phase protein structure**; Brielle L Van Orman[1]; Ryan R. Julian[1]; *[1]University of California, Riverside, Riverside, CA*

MP 241 **Mechanism and application of mass spectrometry fragment generation of B-type procyanidin dimers**; Kuok Fai Li[1]; Pai-Chi Syue[1]; Yao-Yuan Chuang[2]; Kuo-Lung Ku[1]; *[1]National Chiayi University, Chiayi City, Taiwan; [2]National University of Kaohsiung, Kaohsiung City, Taiwan*

MP 242 **Effect of "Fixed" Negative Charges in Peptide Anion Tandem Mass Spectrometry**; Teresa Lee[1]; Steven A. DeFiglia[1]; Kristina Håkansson[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 243 **Unraveling the Mysteries of Intrinsic Electron-Based Fragmentation of Cytochrome c: Insights from Species Variability**; Sarah Brandner[1]; Tanja Habeck[1]; Frederik Lermyte[1]; *[1]Technical University of Darmstadt, Clemens-Schöpf-Institute for Organic Chemistry and Biochemistry, Darmstadt, Germany*

MP 244 **Revisiting Rayleigh Instability: Unveiling the Fission Dynamics of Charged Aqueous Nanodrops Using Charge Detection Mass Spectrometry**; Veena S Avadhani[1]; Zachary M Miller[1]; Matthew S McPartlan[1]; Evan R Williams[1]; *[1]University of California, Berkeley, Berkeley, CA*

MP 245 **Investigating the Utility of Ion Mobility-Enhanced Multistep Collisional Activation for Free Radical Initiated Peptide Sequencing (FRIPS)**; Kemi E. Osho[1]; Nicholas B. Borotto[1]; *[1]University of Nevada, Reno, RENO, NV*

MP 246 **Characterizing HDACi Interactions with Platinum by Collision-Induced Dissociation Tandem Mass Spectrometry**; Rabeya Bosri[1]; Qinliang Zhao[2]; *[1]University of the pacific, Stockton, CA; [2]University of The Pacific, Stockton, CA*

MP 247 **Analysis of surface-induced dissociation of large droplets formed by ESI in wall collisions via molecular dynamics simulations**; Michelle Rajkovic[1]; Walter Wißdorf[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

MP 248 **Complex-Up Characterization of the Ribosome by Infrared Multiphoton Dissociation and Charge Detection Mass Spectrometry**; Sachin Tennakoon[1]; Mashiyat Mubassera[1]; Jared B. Shaw[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

FUNDAMENTALS: ION STRUCTURE/ENERGETICS/REACTIONS

249-264

MP 249 **Thermochemical studies of Tetraglycine using Collision Induced Dissociation via Guided Ion Beam Mass Spectrometry**; Evan H Perez[1]; Brandon C. Stevenson[1]; Peter B. Armentrout[1]; [1]*University of Utah, Salt Lake City, UT*

MP 250 **Elucidation of Saturated Hydrocarbon-derived Ketene and Acylium Ions Using Gas Chromatography Atmospheric Pressure Chemical Ionization High Resolution Mass Spectrometry**; Lindsay P Brown[1]; Joshua B. Powers[1]; Shawn R. Campagna[1]; [1]*University of Tennessee Knoxville Chemistry Dept., Knoxville, TN*

MP 251 **Dehydrogenation of N-Heterocycles by [Fp]+and [CpFe(CO)]+**; Robert S King[1]; Richard O'Hair[2]; Allan Canty[3]; John Sailor[1]; Victor Ryzhov[1]; [1]*Northern Illinois University, Dekalb, IL;* [2]*The University of Melbourne, Melbourne, Australia;* [3]*University of Tasmania, Hobart, Australia*

MP 252 **Optimizing Differentiation of Glycosyl Phosphate Isomers via Tandem Mass Spectrometry: Efficacy of Quasimolecular Ion vs. Fragmentation Patterns vs. Survival Yields**; Nicholas M. R. Frieler[1, 2]; Mary T Rodgers[3]; [1]*Wayne State University, Detroit , MI;* [2]*University of Michigan, Ann Arbor, Michigan;* [3]*Wayne State University, Detroit, MI*

MP 253 **EffectiveAcidities of Isomeric Asp-PolyPro Peptides in the Gas-Phase and in Solution**; Kim Harvey[1]; Yadwinder Singh Mann[1]; Drew Wessels[1]; Carmen Ochoa[1]; Jianhua Ren[1]; [1]*University of the Pacific, Stockton, CA*

MP 254 **Ion Mobility Mass Spectrometry Reveals Changes in the Size of Metal Chalcogenide Clusters Induced by Atom-by-atom Incorporation**; Xilai Li[1]; Hong Fang[2]; Dylan Forbes[1]; Habib Ranjbar Gholipour[1]; Puru Jena[3]; Julia Laskin[1]; [1]*Purdue University Department of Chemistry, West Lafayette, IN;* [2]*Department of Physics, Rutgers University, Camden, NJ;* [3]*Department of Physics, Virginia Commonwealth University, Richmond, VA*

MP 255 **Real-time identification and quantitation of ethylene oxide through selective gas-phase ion-molecule chemistry**; Stefan J Swift[1, 2]; Kseniya Dryahina[1]; Ann-Sophie Lehnert[3]; Nicholas Demarais[4]; Vaughan S. Langford[4]; Mark J. Perkins[5]; Leslie P. Silva[6]; Maroua Omezzine Gnioua[1, 7]; Patrik Spanel[1]; [1]*J Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic;* [2]*Current Affiliation: University of Oslo, Oslo, Norway;* [3]*Syft Technologies, Darmstadt, Germany;* [4]*Syft Technologies, Christchurch, New Zealand;* [5]*Element Lab Solutions, Cambridge, United Kingdom;* [6]*Syft Technologies, Anaheim, CA;* [7]*Charles University, Prague, Czech Republic*

MP 256 **Gas-phase Acidity of D/L-Cysteine-Containing Oligopeptides by Computational and Mass Spectrometry Studies**; Shiyuan Wang[1]; Yuntao Zhang[1]; Jianhua Ren[1]; [1]*University of the Pacific, Stockton, CA*

MP 257 **Elucidation of the Zn(II) affinity of a peptide model of a Zinc finger motif from competitive threshold collision-induced dissociation**; Richmond A Adomako[1]; Michael B Owusu[2]; Laurence A Angel[2]; [1]*Texas A&M University-Commerce, Commerce, TX;* [2]*Texas A&M University - Commerce, Commerce, TX*

MP 258 **Investigating the Structures of the C4H7+ Cation by Cryogenic Infrared (IR) Action Spectroscopy and Electronic Structure Methods**; Maleesha T Fernando[1]; Miyuru M Wellalage[1]; Katja Ober[2]; América Y Torres-Boy[2]; Madeline Schultz[1]; Gert von Helden[2]; Daniel A Thomas[1]; [1]*University of Rhode Island Chemistry Department, Kingston, Rhode Island;* [2]*Fritz Haber Institute of the Max Planck Society, Berlin, Germany*

MP 259 **Nitrile Imines as Novel Photo-Cross-Linkers for Peptides and Oligonucleotides in Gas-Phase Ions**; Jiahao Wan[1]; Marianna Nytka[2]; Haocheng Qian[3]; Kim Vu[3]; Karel Lemr[2, 4]; František Tureček[3]; [1]*University of Washington, Seattle, WA;* [2]*Department of Analytical Chemistry, Faculty of Science, Palacky University, 17. listopadu 12, Olomouc, Czech Republic;* [3]*University of Washingon, Seattle, WA;* [4]*Institute of Microbiology of the Czech Academy of Sciences, Prague, Czech Republic*

MP 260 **pH dependence of Ni(II) and Zn(II) affinities of alternative metal binding peptides from competitive threshold collision-induced dissociation**; Laurence Angel[1]; Perfect Asare[1]; Kwabena N. Senyah[1]; Jonathan D. Wilcox[1]; Jovany Morales[1]; Riccardo Spezia[2]; [1]*Texas A&M University - Commerce, Commerce, TX;* [2]*Laboratoire de Chimie Theorique, Sorbonne Universite, Paris, France*

MP 261 **Towards Annotating the Structural Heterogeneity of Model Proteins Using Gas-Phase Hydrogen/Deuterium Exchange Within an Atmospheric Pressure IM-Orbitrap Platform**; Haley M Schramm[1]; Brian H Clowers[1]; [1]*Washington State University Department of Chemistry, Pullman, WA*

MP 262 **In-Source Reactivity Mass Spectrometry: Revealing Reactive Species through High-Resolution Characterization**; Bessem BRAHIM[1]; Alban HUTEAU[1]; Thierry LEGOUPIL[1]; [1]*Shimadzu, Noisiel, France*

MP 263 **Further Exploration of the Intrinsic Behavior of U(III) and U(IV) Complex Ions: Reactions with Iodoethane, Iodopropanes and Vinyl Iodide**; Samuel J Lenze[1]; Michael J Van Stipdonk[1]; [1]*Duquesne University, Pittsburgh, PA*

MP 264 **Cyanocyclopentadiene Annulated Polycyclic Aromatic Radical Anions: Isomer-specific Negative Ion Photoelectron Spectra and Thermochemistry Cyanoindene and Cyanofluorene Radical Anions**; Wilson Gichuhi[1]; Dushmantha N. Koku Hannadige Abeysooriya[1]; Nolan J White[1]; [1]*Tennessee Tech University, Cookeville, TN*

FUNDAMENTALS: MOLECULAR MODELING/QUANTUM MECHANICAL CALCULATIONS

265-270

MP 265 **Understanding Water Adduction to Lithiated Cannabinoids**; Conner J. Baucom[1]; Shubin Liu[1]; Gary L. Glish[1]; [1]*University of North Carolina at Chapel Hill, Chapel Hill, NC*

MP 266 **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 267 **Accelerating gas-phase simulations of large proteins with the fast multipole model**; Louise J Persson[1]; Erik G Marklund[1]; [1]*Uppsala University, Uppsala, Sweden*

MP 268 **Exploring Oligomerization of Liraglutide: An Integrative Approach Using Ion Mobility Mass Spectrometry, Molecular Dynamics, and Statistic Methods**; Zhenyu Xi[1]; Syuan-Ting Kuo[1]; David H Russell[1]; [1]*TAMU, College Station, TX*

MP 269 **Exploring the Influence of Microsolvation on the Conformational Landscape of Deprotonated Peptides: Computational Investigation of Leucine Enkephalin and Diserinol Isophthalamide**; Nwanne D Banor[1]; Madeline Schultz[1]; Maleesha T Fernando[1]; Miyuru M Madduma Wellalage[1]; Daniel A Thomas[1]; [1]*University of Rhode Island Chemistry Department, Kingston, Rhode Island*

MP 270 **Investigating the Correlation between Bimodal CSDs of a Protein and its Behavior During the Desolvation Process using Molecular Dynamics Simulations**; Samira Hajian Foroushani[1]; Daud Sharif[1]; Stephen J Valentine[1]; [1]*West Virginia University, Morgantown, WV*

GLYCOMICS

271-296

MP 271 **Ultra-Sensitive LC-MRM Based Method for Rapid and High-Throughput Screening of Sugar Phosphate Isomers in Cell Culture**; Fatemeh Mousavi[1]; Vijay Kumar[2]; Jingwen Yue[1, 3]; Dan Su[1, 3]; [1]*HD Biosciences, San Diego, CA;* [2]*University of Colorado, Aurora, CO;* [3]*WuXi AppTec, SAN DIEGO, California*

MP 272 **De novo determination of fucose linkages in N-glycans and the unusual fucosylated N-glycans in insect**; Chi-Kung Ni; *Academia Sinica, Taipei, Taiwan*

MP 273 **Comparative Analysis of Milk Oligosaccharides via LC-MS: Assessing production in milk from globally distributed breeds and endangered Nordic cows**; Yu Wang[1]; Yu-Ping Huang[1]; Daniela Barile[1]; Heidi Leskinen[2]; Päivi Soppela[3]; Anne Tuomivaara[3]; *[1]Food Science and Technology, University of California, Davis, California; [2]Natural Resources Institute Finland, Jokioinen, Finland; [3]University of Lapland, Arctic Centre, Rovaniemi, Finland*

MP 274 **Lectin-based SP3 Technology Enables N-glycoproteomics Analysis of Low Amount of Samples**; Yueshuai Guo[1]; Zian Huo[1]; Haixia Tu[1]; Xiangzheng Zhang[1]; Xuejiang Guo[1]; *[1]State Key Laboratory of Reproductive Medicine and Offspring Health, Nanjing Medical University, Nanjing, China*

MP 275 **The Integration of Comprehensive Glycomic Profiling and Proteomic Analysis to Discern Unique Quality Attributes in Various Cell Therapeutics**; In-Seok Yeo[1, 2]; Myung Jin Oh[1, 2]; Sol Kim[1, 2]; Jae-Youg Kim[1]; Hyun Joo An[1, 2]; *[1]Chungnam National University, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea*

MP 276 **Deciphering Glycosylation Changes in Glycoengineered Xenograft Models Using Glycocentric-Omics**; Myung Jin Oh[1, 2]; Ji Eun Park[1, 2]; Jae Ho Kim[1, 2]; Joohyun Shim[3]; Kimyung Choi[3]; Hyun Joo An[1, 2]; *[1]Chungnam National Univeristy, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; [3]Optipharm Inc., Chungcheongbuk-do, South Korea*

MP 277 **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[1]; Lingjun Li[2, 3]; *[1]University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

MP 278 **Boosting Quantification of N-Glycans by Enhanced Isobaric Multiplex Reagents for Carbonyl-Containing Compound (SUGAR) Tagging Strategy**; Jingwei Zhang[1]; Zicong Wang[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

MP 279 **From Alpha to Omicron: Comparative O-Glycome Analysis of SARS-CoV-2 Spike Protein S1 by LC-MS/MS**; Parisa Ahmadi[1]; Vishal Sandilya[1]; Peilin Jiang[1]; Oluwatosin Daramola[1]; Judith Nwaiwu[1]; Arvin Saffarian Delkhosh[1]; Mojgan Atashi[1]; Mojibola Fowowe[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

MP 280 **Resolving Isomeric Saccharides using High Performance Liquid Chromatography Coupled to Contained Electrospray Ionization Mass Spectrometry (HPLC-cESI-MS)**; Santosh Raman Acharya[1]; Abraham Badu-Tawiah[1]; *[1]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH*

MP 281 **An Innovative Method for Analyzing IgG Glycosylation Significance inTraumatic Brain Injury**; Sherifdeen B Onigbinde[1]; Joy Solomon[1]; Vishal Sandilya[1]; Oluwatosin E Daramola[1]; Mojibola Fowowe[1]; Moyinoluwa Adeniyi[1]; Firas Kobeissy[2]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas; [2]Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA*

MP 282 **In vitro Stable Labeling (GlyProSILC) of Mitochondria Glycans and Proteins: Unveiling Hidden Sugars in Organelles**; Judith Ijeoma Nwaiwu[1]; Peilin Jiang[1]; Oluwatosin E Daramola[1]; Miriam Mechref[1]; Odunayo O. Oluokun[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

MP 283 **Mass Spectrometry-Based N-Glycan Profiling of the Crustacean Neuroendocrine System**; Angel E. Ibarra[1]; Jingwei Zhang[1]; Wenxin Wu[1]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [2]University of Wisconsin-Madison School of Pharmacy, Madison, WI*

MP 284 **Developing novel in-house packed diamond column for separation of polysaccharides based on theoretical predication**; Jyun-Ting Lin[1, 2]; Chein-Hung Chen[1]; Ya-Ping Lin[1]; Chia-Lin Wu[1]; Jung-Lee Lin[1]; *[1]Genomics Research Center Academia Sinica, Taipei, Taiwan; [2]National Cheng Kung University, Tainan, Taiwan*

MP 285 **Proteomic Insights into the Interplay between p97 and N-Glycan Profiles in Cancer Cells**; Chia Yen Liew[1, 2]; Tsui-Fen Chou[1, 2]; *[1]Biology and Biological Engineering, California Institute of Technology, Pasadena, CA; [2]Proteome Exploration Laboratory, Beckman Institute, California Institute of Technology, Pasadena, CA*

MP 286 **Profiling N- and O-glycosylation in pancreatic juices for earlier detection of pancreatic cancer among high-risk individuals**; Yuri Van Der Burgt[1]; Tao Zhang[1]; Jihane Meziani[2]; Oleg A. Mayboroda[1]; Djuna L. Cahen[2]; Gwenny M. Fuhler[2]; Maikel P. Peppelenbosch[2]; Marco J. Bruno[2]; Manfred Wuhrer[1]; *[1]Leiden University Medical Center, Leiden, Netherlands; [2]Erasmus Medical Center, Rotterdam, Netherlands*

MP 287 **Defining the Severity of Traumatic Brain Injury Using LC-MS/MS Glycomics of Biofluids**; Joy O Solomon[1]; Cristian D Gutierrez-Reyes[1]; Sherifdeen B Onigbinde[1]; Moyinoluwa Adeniyi[1]; Mojibola Fowowe[1]; Md Mostofa Al Amin Bhuiyan[1]; Oluwatosin E Daramola[1]; Judith Ijeoma Nwaiwu[1]; Firas Kobeissy[2]; Stefania Mondello[3]; Ava M Puccio[4]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA; [3]Department of Biomedical and Dental Sciences and Morphofunctional Imaging, University of Messina, Messina, Italy; [4]Department of Neurological Surgery, University of Pittsburgh, Pittsburgh, PA*

MP 288 **Paediatric IgA Vasculitis: An LC-FAIMS-EThcD-MS/MS O-glycan pipeline**; Andrew Chetwynd[1]; Claire E. Eyers[2]; Louise Oni[2, 3]; *[1]University of Liverpool, Liverpool, United Kingdom; [2]Liverpool University, Liverpool, United Kingdom; [3]Alder Hey Children's Hospital, Liverpool, United Kingdom*

MP 289 **Glycome Profiling of Small Extracellular Vesicle N-glycans as Disease Biomarkers: A Traumatic Brain Injury Case Study**; Esther O. Oji[1]; Mojibola Fowowe[1]; Moyinoluwa Adeniyi[1]; Ayobami Oluokun[1]; Oluwatosin E Daramola[1]; Angel J Garcia[1]; Cristian Gutierrez-Reyes[1]; Firas Kobeissy[2]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA*

MP 290 **Serum N-Glycan Alterations in Rats Chronically Exposed to Glyphosate-Based Herbicide**; Favour M Chukwubueze[1]; Moyinoluwa Adeniyi[1]; Cristian D Gutierrez-Reyes[1]; Jesús Chávez-Reyes[2]; Bruno A Marichal-Cancino[2]; Joy O Solomon[1]; Mojibola O Fowowe[1]; Sherifdeen B Onigbinde[1]; Md Mostofa Al Amin Bhuiyan[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Department of Physiology and Pharmacology, Center of Basic Sciences, Universidad Autónoma de Aguascalientes, Aguascalientes, Mexico*

MP 291 **Characterization and quantification of mono/oligo/polysaccharides naturally occurring in pomegranate mesocarp via microfluidic chip-Q-TOF and QQQ platforms**; Han Peng[1]; Daniela Barile[1]; Nitin Nitin[1]; Bruna Paviani[1]; Yu-Ping Huang[1]; Nitya Raisinghani[1]; *[1]UC Davis, Davis, CA*

MP 292 **Advancing Glycomics in High Grade Gliomas: A MIBI-TOF and MALDI Imaging Integrated Approach**; Mikaela Ribi[1]; Hadeesha Piyadasa[1]; Davide G. Franchina[1]; Ke Leow[1]; Meelad Amouzgar[1]; Benjamin Oberlton[1]; Richard R Drake[2]; Carolyn R. Bertozzi[1]; Sean Bendall[1]; Mike Angelo[1];

[1]Stanford University, Stanford, CA; [2]Medical University of South Carolina, Charleston, SC

MP 293 **A novel, high-accuracy glucose-unit based N-glycan retention library and peak assignment tool for compound identification in LC or LC/MS data**; Randall Robinson[1]; Tom Rice[1]; Steven Mast[1]; Aled Jones[1]; Oscar Potter[2]; *[1]Agilent Technologies, Folsom, CA; [2]Agilent Technologies, Santa Clara, CA*

MP 294 **Mechanistic and Quantitative Insights into Protein Interactions with Glycosphingolipids in Model Membranes**; Linh Nguyen[1]; Ling Han[1]; Elena N. Kitova[1]; Jianing Li[1]; John S. Klassen[1]; *[1]Department of Chemistry, University of Alberta, Edmonton, AB*

MP 295 **Rapid LC-MS Glycan Analysis Enabling Accurate Glycan Profiling for Antibody Molecules in Cell Line Development**; Sakshi Gautam[1]; YenRu Pan[1]; Tawnya Flick[1]; *[1]Gilead Sciences Inc, Oceanside, CA*

MP 296 **Discovering biomarkers in host-microbe interactions in Bacterial Vaginosis**; Yasmine Bouchibti[1]; Carlito B. Lebrilla[2]; Amanda L Lewis[3]; *[1]UC Davis Graduate Studies, Davis, CA; [2]UC Davis, Davis, CA; [3]UC San Diego, La Jolla, CA*

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MP 297 **Towards Selective Removal of Unwanted Proteins under H/D Exchange Quench Conditions**; Kent Robert Vosper[1]; Madison Turner[1]; Algirdas Velyvis[1]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON*

MP 298 **Towards the development of an automated in vivoHDX system to probe conformational dynamics of membrane proteins**; Juan P Rincon Pabon[1]; Charlotte Guffick[1]; Argyris Politis[1]; *[1]The University of Manchester, Manchester, United Kingdom*

MP 299 **A novel HDX-MS platform for analyzing protein interactions in complex biological systems**; Joel B Langford[1]; Mulin Fang[1]; Oliver Wu[1]; Kellye Cupp-Sutton[2]; Kathleen Norris[3]; Judith James[3, 4, 5]; Kenneth Smith[3]; Si Wu[2]; *[1]University of Oklahoma, Norman, OK; [2]University of Alabama, Tuscaloosa, AL; [3]Department of Arthritis and Clinical Immunology, Oklahoma Medical Research Foundation, Oklahoma City, OK; [4]Department of Microbiology and Immunology, Oklahoma Medical Research Foundation, Oklahoma City, OK, United States, Oklahoma City, OK; [5]Department of Medicine and Pathology, Oklahoma Medical Research Foundation, Oklahoma City, OK, United States, Oklahoma City, OK*

MP 300 **Advancements in MALDI for Hydrogen Deuterium Exchange Mass Spectrometry: A Systematic Evaluation**; Taylor A Murphree[1]; Miklos Guttman[2]; *[1]University of Washington, Seattle, WA; [2]University of Washington, Seattle, WA*

MP 301 **HDXWizard: a software for customizable hydrogen deuterium exchange data visualization**; Zachary A. Cohen[1]; Bindu Y. Srinivasu[1]; Daniele Peterle[1]; John R. Engen[1]; Thomas E. Wales[1]; *[1]Northeastern University, Boston, MA*

MP 302 **Scaling HX-DIA to high throughput experimentation by replacing manual validation with statistical methods**; Vladimir Sarpe[1]; Jürgen Claesen[2]; František Filandr[1]; Arthur Semague[1]; Joey Sheff[3]; David C. Schriemer[1]; *[1]University of Calgary, Calgary, AB; [2]Amsterdam University Medical Center, Amsterdam, Netherlands; [3]National Research Council of Canada, Ottawa, ON*

MP 303 **Leveraging cyclic ion mobility to enhance hydrogen/deuterium exchange-mass spectrometry analyses of membrane proteins within native-like lipid environments**; Damon Griffiths[1]; Malcolm Anderson[2]; Keith G Richardson[2]; Charlotte Guffick[1]; Satomi Inaba-Inoue[3]; Konstantinos Beis[3]; Mike Morris[2]; Kevin Giles[2]; Argyris Politis[1]; *[1]University of Manchester, Manchester, United Kingdom; [2]Waters Corporation, Manchester, United Kingdom; [3]Imperial College London, London, United Kingdom*

MP 304 **Optimization of Instrument Parameters for HX-DIA with AutoHX**; Maryam Hassannia[1]; František Filandr[1]; David C. Schriemer[1]; *[1]University of Calgary, Calgary, AB*

MP 305 **Determining EX1 protein unfolding kinetics in library scale HDX experiments**; Jane Thibeault[1]; Állan J. R. Ferrari[1]; Gabriel Rocklin[1]; *[1]Northwestern University, Feinberg School of Medicine, Chicago, IL*

MP 306 **Streamlined Software Approach for Controlling Modules in a Mass Spectrometer**; Francis E. Godfrey[1]; Michael Eller[1]; *[1]Cal State Northridge, Northridge, CA*

MP 307 **Reducing gas-phase hydrogen/deuterium scrambling on a QTOF Mass Spectrometer equipped with electron activated dissociation (EAD) fragmentation technology**; Joseph Anacleto[1]; Ebadullah Kabir[2]; Yves LeBlanc[3]; Cristina Lento[2]; Derek J. Wilson[2]; *[1]Emeritus, Brampton, ON; [2]York University, Toronto, ON; [3]SCIEX, Concord, ON*

MP 308 **Probe the Protein Conformation using Top-down Hydrogen Exchange Mass Spectrometry at Higher Resolution with Electron Transfer Dissociation**; Yuqi Shi[1]; Graeme McAlister[1]; Rosa Viner[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

H/D EXCHANGE: PROTEIN STRUCTURE/FUNCTION
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MP 309 **HDX-MS insights into the conformational and oligomeric heterogeneity of PafA, the mycobacterial prokaryotic ubiquitin-like protein (Pup) ligase**; Alicia Plourde[1]; Jacquelyn Ogata-Bean[1]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON*

MP 310 **Substrate engagement mechanism of an ATP-independent proteasome activator from Mycobacterium tuberculosis: Insights from HDX and native MS**; Bradley Davis[1]; Algirdas Velyvis[1]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON*

MP 311 **Investigating the role of allostery in the regulation of human mitochondrial ClpP: implications for the treatment of acute myeloid leukemia**; Monica M Goncalves[1]; Adwaith B. B. Uday[2]; Ian Watson[3]; S. Quinn W. Currie[1]; Taylor Forrester[1]; Angelina S. Kim[1]; Algirdas Velyvis[1]; Matthew Kimber[1]; Rima Al-Awar[3]; Natalie Zeytuni[2]; Aaron Schimmer[4]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON; [2]McGill University, Montreal, QC; [3]Ontario Institute for Cancer Research, Toronto, ON; [4]Princess Margaret Cancer Centre, University Health Network, Toronto, ON*

MP 312 **The Unique Advantage of HDX-MS Over Traditional Structural Biology Tools: the Case of the 20S Proteasome Core Particle**; Madison Turner[1]; Samuel E Hoff[2]; Adwaith B. B. Uday[3]; Algirdas Velyvis[1]; Natalie Zeytuni[3]; Massimiliano Bonomi[2]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON; [2]Institut Pasteur, Paris, France; [3]McGill University, Montreal, QC*

MP 313 **A Structural and Dynamic Basis for the Interactions of the Dengue Nonstructural (NS5) Protein with Stem Loop A (SLA)**; Juliet Obi[1]; Kyle C. Kihn[2]; Ally K. Smith[1]; Linfah McQueen[1]; Daniel J. Deredge[1]; *[1]University of Maryland, Baltimore, Baltimore, MD; [2]Georgetown University, Washington Dc, DC*

MP 314 **pH-dependent conformational changes and structural dynamics of Brain-Type Creatine Kinase**; Nolan K McLaughlin[1]; Samantha Gies[2]; Reza Dastvan[2]; Michael Gross[1]; *[1]Washington University in Saint Louis, St. Louis, MO; [2]Saint Louis University School of Medicine, St. Louis, MO*

MP 315 **Characterization of a new class of influenza antibodies by integrating HDX-MS with computational modeling**; Minh H. Tran[1]; Cristina E. Martina[1]; Iuliia M. Gilchuck[2]; James E. Crowe[2, 3, 4]; Jens Meiler[1, 5]; Kevin L. Schey[6]; *[1]Department of Chemistry and Center for Structural Biology, Vanderbilt University, Nashville, TN; [2]Vanderbilt Vaccine Center, Vanderbilt University Medical Center, Nashville, TN; [3]Department of Pediatrics, Vanderbilt University Medical*

Center, Nashville, TN; [4]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; [5]Institute for Drug Discovery, University Leipzig Medical School, Leipzig, Saxony; [6]Department of Biochemistry and Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN

MP 316 **Characterizing the functional role of the C-terminal extension of human mitochondrial ClpP**; S. Quinn W. Currie[1]; Monica M. Goncalves[1]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON*

MP 317 **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[1, 2]; Rohana Liyanage[1, 2]; Isini Ranawake Arachchige[1, 2]; Wesley Stites[1]; Jackson O. Lay[1, 2]; *[1]UNIVERSITY OF ARKANSAS, FAYETTEVILLE, AR; [2]Arkansas Statewide Mass Spectrometry Facility, FAYETTEVILLE, AR*

MP 318 **Comprehensive HDX-MS Analysis is a Key Driver in Lead Selection and Characterization in Pharmaceutical Research**; Cornelia Wagner[1]; Sarah Mundigl[1]; Urs Hanke[1]; Maximiliane Koenig[1]; *[1]Roche Innovation Center Munich (RICM), Roche Pharma Research and Early Development (pRED), Penzberg, Germany*

MP 319 **Analyzing protease inhibitors: A case study on the Coronavirus 3CL protease using an automated rapid screening and HDX-MS**; Jonathan Zöller[1]; Frederic Farges[2]; Barbara Rathmann[1]; Joshua Vollrath[1]; Nadide Altincekic[3, 4]; Kristina Desch[5]; Jakob Meier-Credo[1]; Harald Schwalbe[3, 4]; Ulrich Mrowietz[6]; Julian D. Langer[1, 5]; *[1]Max Planck Institute of Biophysics, Frankfurt, Germany; [2]Institute of Pharmaceutical Chemistry, Johann Wolfgang Goethe University, Frankfurt am Main, Germany; [3]Center for Biomolecular Magnetic Resonance (BMRZ), Institute for Organic Chemistry and Chemical Biology, Goethe University, Frankfurt am Main, Germany; [4]Institute for Organic Chemistry and Chemical Biology, Goethe University, Frankfurt am Main, Germany; [5]Max Planck Institute for Brain Research, Frankfurt, Germany; [6]Dept. of Dermatology, University Medical Center Schleswig-Holstein, Kiel, Germany*

MP 320 **Epitope mapping and protein dynamics analysis by HDX-MS to characterize the antigenicity maturation effect of SARS CoV-2 Beta spike protein**; Shaolong Zhu[1]; Lisa Szymkowicz[1]; Jason Szeto[1]; Fernando Salvador Ausar[1, 2]; Andrew James[1]; Michael Leach[1]; *[1]Sanofi, Toronto, ON; [2]Vaxcyte, San Carlos, CA*

MP 321 **Unraveling Variations in the Dynamic Binding of PD1 between Toripalimab and other Commercial PD-1 Monoclonal Antibodies through HDX-MS Analysis**; Bin Yu[1]; Glen Young[1]; *[1]coherus bioscience, Camarillo, CA*

MP 322 **Structural basis of DNMT3A oligomeric states in acute myeloid leukemia revealed by hydrogen-deuterium exchange (HX) and cross-linking (XL) mass spectrometry**; Shaunak Raval[1]; Emma Garcia[2]; Keith Rivera[1]; Maya Virshup[1]; Brian B. Liau[1, 2]; Steven A. Carr[1]; Malvina Papanastasiou[1]; *[1]Broad Institute, Cambridge, MA; [2]Harvard University, Cambridge, MA*

MP 323 **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[1, 2]; Rohana Liyanage[1, 2]; Motolani O Matthew[1, 2]; Wesley Stites[1]; Jackson O. Lay[1, 2]; *[1]UNIVERSITY OF ARKANSAS, FAYETTEVILLE, AR; [2]Arkansas Statewide Mass Spectrometry Facility, FAYETTEVILLE, AR*

MP 324 **HDX-MS of surface-bound IgM provides insight into complement cascade activation**; Charles Mundorff[1]; Malika Hale[1]; Adian Valdez[1]; Lauren Carter[1]; Neil King[1]; David J Rawlings[1]; Marion Pepper[1]; Miklos Guttman[1]; *[1]University of Washington, Seattle, WA*

MP 325 **Beyond epitope mapping: combining solid-state NMR and structural mass spectrometry to gain new insights for precision biotech development**; Francesca Sacco[1]; Angela Capolupo[2]; Sofia Petrocchi[3]; Jonathan Zöller[4]; Linda Cerofolini[1, 5]; Julian D. Langer[4, 6]; Fabio Baroni[3]; Marco Fragai[1, 5, 7]; *[1]Magnetic Resonance Center (CERM), University of Florence, Sesto Fiorentino (FI), Italy; [2]Analytical Development & Innovation - NBE, Merck Serono S.p.a, Guidonia (Rome), Italy; [3]Analytical Development & Innovation - NBE, Merck Serono S.p.a, Guidonia (Rome), Italy; [4]Max Planck Institute of Biophysics, Frankfurt, Germany; [5]Consorzio Interuniversitario Risonanze Magnetiche di Metalloproteine (CIRMMP), Sesto Fiorentino (FI), Italy; [6]Max Planck Institute for Brain Research, Frankfurt, Germany; [7]Department of Chemistry "Ugo Schiff", University of Florence, Sesto Fiorentino (FI), Italy*

MP 326 **Hydrogen Deuterium Exchange Mass Spectrometry of the CheW Coupling Protein in E.coli Chemoreceptor Complexes**; Isabella J Jankowski[1]; Thomas Tran[1]; Lynmarie K. Thompson[1, 2]; Steve Eyles[2]; *[1]Department of Chemistry, University of Massachusetts Amherst, Amherst, MA; [2]Department of Biochemistry and Molecular Biology, University of Massachusetts Amherst, Amherst, MA*

MP 327 **Impact of clinically approved BTK inhibitors on full-length BTK conformation and analysis of the development of BTK resistance mutations**; Thomas E. Wales[1]; Raji E. Joseph[2]; Sandrine Jayne[3]; Robert G. Britton[3]; D. Bruce Fulton[2]; John R. Engen[1]; Martin J.S. Dyer[3]; Amy H. Andreotti[2]; *[1]Northeastern University, Boston, MA; [2]Iowa State University, Ames, IA; [3]University of Leicester, Leicester, United Kingdom*

MP 328 **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[1]; Zhongping Yao[2]; *[1]the Hong Kong Polytechnic University, Kowloon, Hong Kong; [2]The Hong Kong Polytechnic University, Kowloon, Hong Kong*

MP 329 **Combination of HDX-MS and MD Simulations Identified Closed Conformation of the Full-Length Bcl-2**; Miray Turk[1]; Umut Cagan Ucar[1]; Baran Dingiloglu[1]; Yagiz Akbas[1]; Gizem Dinler Doganay[1]; *[1]Istanbul Technical University, Istanbul, Turkey*

MP 330 **HDX-MS reveals binding of a neutralizing antibody to TNFα allosterically interferes with its binding to TNFR1**; Christopher A. Haynes[1]; Theodore R. Keppel[1]; John R. Barr[1]; Dongxia Wang[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

MP 331 **Native MS and HDX Characterization of the Mechanism of GSTP1 Protein Glutathionylation**; Xinyi Cynthia Kuang[1]; Heather Benedict-Hamilton[2]; Marta Zurawska[2]; Andrzej Krezel[2]; Jason M Held[2]; Michael L. Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

MP 332 **Conformational Dynamics of Glucokinase and Modulation by a Molecular Activator as Characterized by Hydrogen Deuterium Exchange Mass Spectrometry**; Bindu Y. Srinivasu[1]; Michelle S. Prew[2]; Gregory H. Bird[2]; Nika N. Danial[3]; Loren D. Walensky[2]; John R. Engen[1]; Thomas E. Wales[1]; *[1]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; [2]Department of Pediatric Oncology and the Linde Program in Cancer Chemical Biology, Dana-Faber Cancer Institute, Boston, MA; [3]Departments of Cancer Biology and Medical Oncology, Dana-Farber Cancer Institute, Boston, MA*

MP 333 **Mapping Epitopes on Borrelia burgdorferiOuter Surface Proteins by Hydrogen Deuterium Exchange Mass Spectrometry (HDX-MS)**; Clint Vorauer[1]; Beatrice Muriuki[2]; David Vance[3]; Michael Rudolph[4]; Lisa Cavacini[5]; NIcholas Mantis[6]; Miklos Guttman[1]; *[1]University of Washington - Medicinal Chemistry, Seattle, Washington; [2]University of Massachusetts Boston, Boston, Massachusetts; [3]University* *at Albany, State University of New York, Albany, New York; [4]New York Structural Biology Center, New York, New York; [5]University of Massachusetts Boston, Boston, MA; [6]New York State Department of Health, Albany, New York*

MP 334 **MD simulations, mass spectrometry and other biophysical techniques elucidate stabilising features of a nanobody against an HIV capsid**; Valentina Faustinelli[1]; Eva Illes-Toth[2]; Paul Dalby[1]; *[1]UCL, London, United Kingdom; [2]LGC, London, United Kingdom*

MP 335 **Exploring PF4 Dynamics in Thrombocytopenia: Insights from Hydrogen-Deuterium Exchange Mass Spectrometry**; Yi Du[1]; Daniel Heron[1]; Igor A. Kaltashov[1]; *[1]University of Massachusetts-Amherst, Amherst, MA*

MP 336 **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[1]; Cristina Lento[1]; Derek J. Wilson[1]; Mart Ustav Jr. [2]; *[1]York University, Toronto, ON; [2]Icosagen Cell Factory OÜ, Tartu, Estonia*

MP 337 **Structural dynamics of botulinum neurotoxin type A from hydrogen/deuterium exchange mass spectrometry**; Heather Bottomley[1]; David Spencer[2]; Rick Beardmore[2]; Rachel Bostock[2]; Jonathan Phillips[1]; *[1]University of Exeter, Exeter, United Kingdom; [2]Ipsen Biopharm, Wrexham, United Kingdom*

MP 338 **Characterizing Conformational Dynamics of In Vitro Hyperphosphorylated Human Tau by Time-resolved Hydrogen/Deuterium Exchange Mass Spectrometry**; Ayesha Chaudhry[1]; Derek J. Wilson[1]; *[1]York University, Toronto, ON*

MP 339 **Standardization of HDX-MS Paratope Mapping Conditions for Monoclonal Antibodies using a Range of Acidic Proteases**; Dominic Narang[1]; Konrad Celejewski[1]; *[1]Rapid Novor, Kitchener, Ontario*

IMAGING MS: PHARMACEUTICALS, METABOLITES, LIPIDS, AND GLYCANS I

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MP 340 **Revolutionizing Spatial Dermatology: Investigating Sunfilter Efficacy on Reconstructed Human Epidermis with AP-MALDI MSI Metabolomics and Dedicated Data Analysis Software**; Sara Tortorella[1]; Maureen Feucherolles[2]; Giulia Sorbi[1]; Giuseppe Arturi[1]; Sue Kennerley[3]; Gilles Frache[2]; Ismael Zamora[4]; *[1]Mass Analytica, S.L, Bettona, Italy; [2]Luxembourg Institute of Science and Technology, Molecular and Thermal Analysis, Belvaux, Luxembourg; [3]K R Analytical, Sandbach, United Kingdom; [4]Mass Analytica, S.L, Sant Cugat del Vallés, Spain*

MP 341 **Visualisation and quantitation of drug/metabolites by sensitive and fast targeted DESI imaging TQ system**; Emmanuelle Claude[1]; Ross Chawner[1]; Nathalie Delallee[2]; Stephanie Molez[2]; Gregory Nicolas[2]; Joanne Ballantyne[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Bioprojet Biotech, Saint Gregoire, France*

MP 342 **Lessons learnt from the Cancer Grand Challenge Rosetta Project– Metabolic Imaging at Scale**; Rory Thomas Steven[1]; Alex Dexter[1]; Ariadna Gonzalez[1]; Bin Yan[1]; Caroline Pollard[1]; Janella Marie De Jesus[1]; Greg McMahon[1]; Simon Barry[2]; Kevin Brindle[3]; George Poulogiannis[4]; Richard Goodwin[2]; Mariia Yuneva[5]; Owen Sansom[6]; Josephine Bunch[1, 7]; *[1]National Physical Laboratory, London, United Kingdom; [2]AstraZeneca, Cambridge, United Kingdom; [3]Cancer Research UK Cambridge Institute, University of Cambridge, Cambridge, United Kingdom; [4]Institute for Cancer Research, London, United Kingdom; [5]Francis Crick Institute, London, United Kingdom; [6]CRUK Scotland Institute, Glasgow, United Kingdom; [7]Imperial College London, London, United Kingdom*

MP 343 **Spatially Resolved Metabolomics Reveals Tissue-Specific Metabolic Changes in the Kidney and Bladder after Cisplatin Treatment**; Jephte Akakpo[1]; Erika Abbott[2]; Ben Woolbright[3]; Bindesh Shrestha[4]; Cory Scanlan[4]; Dennis Karote[4]; John Taylor[2, 3]; *[1]Department of Pharmacology, Toxicology & Therapeutics, University of Kansas Medical Center, Kansas City, KS; [2]Department of Urology, University of Kansas Medical Center, Kansas City, KS; [3]Department of Cancer Biology, University of Kansas Medical Center, Kansas City, KS; [4]Waters Corporation, Milford, Massachusetts*

MP 344 **Spatial Mapping of Ether Lipids in Tissue via MALDI TIMS Imaging Mass Spectrometry: Characterization of Biomarkers of Peroxisomal Disorders**; Melanie J Campbell[1]; Erin H. Seeley[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

MP 345 **Skin and the Hair Cycle–Spatial Lipidomics Analysis of the Dermis and Epidermis as a Function of the Adipokine Adiponectin**; Katarzyna Walendzik[1]; Eii-Chi Matsuo[2]; Jeff Dahl[3]; Toshiya Matsubara[3]; Shinichi Yamaguchi[2]; Jannine I. Gamayot[1]; Philipp E Scherer[1]; Ruth Gordillo[1]; *[1]UTSouthwestern Medical Center, Dallas, TX; [2]Shimadzu Corporation, Kyoto, Japan; [3]Shimadzu Scientific Instruments, Columbia, MD*

MP 346 **Mass Spectrometry Imaging Reveals Alterations in Protein and N-Glycan Molecular Signatures in Endometriosis Tissues**; Monica Lin[1]; Erin H. Seeley[2]; Suzanne Ledet[3]; Christina Salazar[4]; Michael T. Breen[4]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Houston, Texas; [2]University of Texas at Austin, Austin, Texas; [3]Ascension Seton Medical Center, Department of Pathology, Austin, Texas; [4]The University of Texas at Austin Dell Medical School, Department of Women's Health, Austin, Texas*

MP 347 **Multimodal Mass Spectrometry Imaging of Uveal Melanoma Multi-Cellular Tumour Spheroids to Investigate Key Metabolomic Biomarkers**; Georgia M Millard[1]; Neil A Cross[1]; Karen Aughton[2, 3]; Helen Kalirai[2, 3]; Laura M Cole[1]; *[1]Sheffield Hallam University, Sheffield, United Kingdom; [2]University of Liverpool, Liverpool, United Kingdom; [3]Liverpool Ocular Oncology Research Group, Liverpool, United Kingdom*

MP 348 **Development of MALDI-MSI methods to detect and visualize new TB regimen drugs within TB lesions**; Bandana Bera[1]; Prem Shankar[1]; Jenny Myrick[2]; Meredith Bacci[2]; David Brown[2]; Arnold Louie[2]; George Drusano[2]; Brendan Prideaux[1]; *[1]University Of Texas Medical Branch, Galveston, TX; [2]University of Florida, Department of Medicine, Orlando, FL*

MP 349 **Investigation of Microbial Metabolites and Their Potential for Impact in Early Life Immune System Development**; Troy R Scoggins IV[1]; Julia Flores[2, 3]; Joseph P. Zackular[4, 5]; Michael A. Silverman[3, 4]; Boone M. Prentice[1]; *[1]Department of Chemistry, University of Florida, Gainesville, FL; [2]Department of Pediatrics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [3]Division of Infectious Disease, Children's Hospital of Philadelphia, University of Pennsylvania, Philadelphia, PA; [4]Division of Protective Immunity, Children's Hospital of Philadelphia, Philadelphia, PA; [5]Department of Pathology and Laboratory Medicine, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA*

MP 350 **MALDI mass spectrometry imaging reveals highly localized phosphatidylcholine metabolism alterations in pancreatic tumor tissues in response to gemcitabine treatment**; Nav Raj Phulara[1]; Chiaki Tsuge Ishida[2]; Peter J. Espenshade[2, 3]; Herana Kamal Seneviratne[1]; *[1]Department of Chemistry and Biochemistry, University of Maryland, Baltimore County, Baltimore, MD; [2]Department of Cell Biology, The Johns Hopkins University School of Medicine, Baltimore, MD; [3]Department of Oncology, The Johns Hopkins University School of Medicine, Baltimore, MD*

MP 351 **Evaluation of anti-ENTPD2 antibody treatment in tumors using MALDI imaging mass spectrometry**; Kerri Grove[1]; Shaila Hoque[1]; Samantha Zaharevitz[2]; Richard Salamone[2]; Deborah Knee[2]; Shu Li[3]; Anhthu Dang[3]; Patrick Rudewicz[1]; *[1]Novartis, Emeryville, CA; [2]Novartis, San Diego, CA; [3]Novartis, Cambridge, MA*

MP 352 **Combining MALDI-IMS and segmentation via autofluorescence to analyze glycan speciation within specific functional tissue units in human organs**; David T. Reeves[1, 2]; Audra M. Judd[1, 3]; Lukasz Migas[4]; Ellie L Pingry[1, 2]; Felipe A Moser[4]; Jamie Allen[1, 3]; Angela R. S. Kruse[1, 2]; Melissa A. Farrow[1, 3, 5]; Raf Van De Plas[1, 3, 4]; Jeffrey M Spraggins[1, 2, 3, 5]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN*

MP 353 **Uncovering lipid heterogeneity in cerebral amyloid angiopathy using MALDI IMS coupled with IF microscopy**; Cody Marshall[1, 2, 3]; Claire F Scott[3, 4, 5]; Lissa Ventura-Antunes[6, 7]; Wilber Romero-Fernandez[7]; Alena Shostak[6, 7]; Lukasz Migas[4, 8]; Madeline E Colley[3, 4, 9]; Martin Dufresne[3, 4, 9]; Raf Van De Plas[3, 4, 8]; Matthew S Schrag[6, 7]; Jeffrey M Spraggins[1, 3, 4, 5, 9, 10]; *[1]Chemical and Physical Biology Program, Vanderbilt University, Nashville, Tennessee; [2]Biomolecular Multimodal Imaging Center, Nashville, Tennessee; [3]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [4]Biomolecular Multimodal Imaging Center, Vanderbilt University, Nashville TN, Nashville, Tennessee; [5]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, Tennessee; [6]Vanderbilt University Medical Center, Nashville, TN; [7]Department of Neurology, Vanderbilt University, Nashville, TN; [8]Delft University of Technology, Delft, Netherlands; [9]Department of Biochemistry, Vanderbilt University, Nashville, TN; [10]Department of Chemistry, Vanderbilt University, Nashville, TN*

MP 354 **Comparison of Antigen Retrieval Techniques to Improve Lipidomic Analysis of Formalin-Fixed/Paraffin-Embedded Tissue in MALDI-MSI Using Canine Sarcoma Samples**; Ziven Noorani[1]; A Colleen Crouch[1]; *[1]University of Tennessee, Knoxville, TN*

MP 355 **Spatial metabolomics reveals accumulation of ceramides and sphingomyelins in motor neurons of lumbar spinal cords in amyotrophic lateral sclerosis**; Guanshi Zhang[1]; Ian M. Tamayo[1]; Stacey Jacoby[2]; Stephen Goutman[2]; Eva L. Feldman[2]; Kumar Sharma[1]; *[1]UT Health San Antonio, San Antonio, TX; [2]University of Michigan-Ann Arbor, Ann Arbor, MI*

MP 356 **Investigating Metabolic Alterations in Neonatal Transgenic Mice Heart with Various Proliferation Capacity using Desorption Electrospray Ionization Mass Spectrometry Imaging**; Sarah Bench[1]; Abou Bakr M. Salama[1]; Tamer M. A. Mohamed[1]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Dept. of Surgery, Houston, Texas*

MP 357 **Applications of Mass Spectrometry-Based Platforms to Advance Drug Discovery Pipeline**; Esther Cheow[1]; U-Ming Lim[1]; Nikhil Tulsian[1]; Matthew Choo[1]; Aaron Zefrin Fernandis[1]; *[1]Target & Pathway Biology, Quantitative Biosciences, MSD, Singapore, Singapore*

MP 358 **Defining lipidomic and metabolic signatures of monomicrobial and dual-species biofilms using MALDI IMS**; Alexis P. Pope[1, 2]; Jeffrey A. Freiberg[3, 4]; Lukasz Migas[5]; Madeline E. Colley[1, 6]; Raf Van De Plas[5]; Eric P. Skaar[3, 7]; Jeffrey M. Spraggins[1, 2, 3, 7, 8, 9, 10]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN; [3]Vanderbilt Institute for Infection, Immunology and Inflammation, Vanderbilt University Medical Center, Nashville, TN; [4]Division of Infectious Diseases, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; [5]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [6]Vanderbilt University, Department of Biochemistry, Nashville, TN; [7]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; [8]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [9]Department of Chemistry, Vanderbilt University, Nashville, TN; [10]Department of Biochemistry, Vanderbilt University, Nashville, TN*

MP 359 **Revealing Spatial Heterogeneity at the Gut Epithelium-Lumen Interface through High-Resolution MALDI-TOF Chemical Imaging**; Jacob Haffner[1]; Gillian Robbins[1]; Soo Hyun Ahn[2]; Tian Autumn Qiu[1]; *[1]Michigan State University, Department of Chemistry, East Lansing, MI; [2]Michigan State University, College of Veterinary Medicine, Department of Pathobiology and Diagnostics Investigation, East Lansing, MI*

MP 360 **Investigating long-term exposure to phthalates in patients with skin abscesses using MALDI FT-ICR MSI**; Temple Andrews[1]; Beita Badiei[2]; Nina Rossa Haddad[2]; Hana Minsky[2]; Yingchao Xue[2]; Luis Garza[2]; Maureen A Kane[1]; *[1]University of Maryland School of Pharmacy, Baltimore, MD; [2]Johns Hopkins University School of Medicine, Baltimore, MD*

MP 361 **Mapping Metabolites in the Human Eye: Integrating High Spatial Resolution MALDI IMS for Insights into Ocular Health**; Ali Zahraei[1, 2]; Martin Dufresne[2, 3]; David M. G. Anderson[2, 3]; Madeline E Colley[1, 2]; Angela R. S. Kruse[1, 2]; Lukasz Migas[4]; Jeffery Messinger[5]; Christine A Curcio[5]; Raf Van De Plas[4]; Kevin L. Schey[2, 3]; Jeffrey M Spraggins[1, 2, 3, 6, 7]; *[1]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Delft University of Technology, Delft, Netherlands; [5]University of Alabama at Birmingham, Birmingham, AL; [6]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; [7]Department of Chemistry, Vanderbilt University, Nashville, TN*

MP 362 **Highly sensitive nano-DESI mass spectrometry imaging of glycolipids using ionization enhancement solvent additives**; Aiming Zheng[1]; Miranda Weigand[2]; Manxi Yang[2]; Julia Laskin[2]; *[1]Purdue University, Department of Chemistry, West Lafayette, IN; [2]Purdue University Department of Chemistry, West Lafayette, IN*

MP 363 **Mass Spectrometry Imaging Analysis Reveals Dysregulated Metabolic Pathways in an Inherited Form of Kidney Disease**; Ian Tamayo[1]; Mengyuan Ge[2]; Alessia Fornoni[2]; Kumar Sharma[1]; *[1]UT Health San Antonio, San Antonio, TX; [2]University of Miami, Miami, FL*

MP 364 **Multiplex and multiomic MS imaging of drugs, metabolites, and immunolabeled pathogenic protein markers within a single tissue section**; Prem Shankar[1]; Reina N Paez[1]; David Beaver[1]; Bandana Bera[1]; Brendan Prideaux[1]; *[1]University of Texas Medical Branch, Galveston, TX*

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MP 365 **Mass spectrometry imaging with spatially resolved omics in mouse brain**; Saira Hameed[1]; Matija Lagator[2]; Daniel Simon[1, 3]; Kenny Robinson[1]; Felicia Green[1]; Bela Paizs[1]; Zoltan Takats[1, 3]; *[1]Rosalind Franklin Institute, Didcot, United Kingdom; [2]Rosalind Franklin Institute, Harwell, United Kingdom; [3]Imperial College London, Hammersmith Hospital, London, United Kingdom*

MP 366 **A comprehensive view of molecular and cellular heterogeneity in S. aureusinfected tissue microenvironments**; Jacqueline M Van Ardenne[1, 2]; Lukasz Migas[2, 3]; Morad C Malek[2, 4]; Roy Lardenoije[5]; Jeffrey A Freiberg[6, 7]; Kyle T Enriquez[7, 8, 9]; Katherine N Gibson-Corley[9]; Angela R.S. Kruse[2, 4]; Melissa A. Farrow[2, 10]; Joana P Gonçalves[5]; Raf Van De Plas[2, 3, 10]; Eric P Skaar[7, 9, 11]; Jeffrey M Spraggins[1, 2, 4, 9, 10]; *[1]Department of Chemistry, Vanderbilt University, Nashville, TN; [2]Mass Spectrometry*

Research Center, Vanderbilt University, Nashville, TN; [3]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [4]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [5]Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands; [6]Division of Infectious Diseases, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; [7]Vanderbilt Institute for Infection, Immunology and Inflammation, Vanderbilt University Medical Center, Nashville, TN; [8]Vanderbilt University Medical Scientist Training Program, Vanderbilt University School of Medicine, Nashville, TN; [9]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; [10]Department of Biochemistry, Vanderbilt University, Nashville, TN; [11]Vanderbilt Institute for Chemical Biology, Vanderbilt University, Nashville, TN

MP 367 **Selective Mapping of Lipids in the Brain using Desorption Electrospray Ionization Coupled with Multiple Reaction Monitoring Tandem Mass Spectrometry**; Marios Georgiadis[1]; Michael Zeineh[1]; Inma Cobos[2]; Jeffrey Nirschl[2]; Xiaowei Vivian Lu[3]; Ryan Leib[3]; Allis Chien[3]; Andrew Baker[4]; *[1]Department of Radiology, Stanford School of Medicine, Stanford, CA; [2]Department of Pathology, Stanford School of Medicine, Stanford, CA; [3]Stanford University Mass Spectrometry, Stanford, California; [4]Waters Corporation, Pleasanton, CA*

MP 368 **A spatial multiomics workflow on a new benchtop MALDI-TOF instrument for deciphering the lipid and expressed protein landscape in tissues**; Janina Oetjen[1]; Corinna Henkel[1]; Ulrike Schweiger Hufnagel[1]; Tobias Boskamp[1]; Sebastian Boehm[1]; Christoph Nordmann[1]; Andree Schuster[1]; Katherine Stumpo[2]; Michael Easterling[2]; Jens Christmann[3]; Andrea Tannapfel[3]; *[1]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; [2]Bruker Scientific, 40 Manning Road, Billerica, MA; [3]Institute for Pathology, Ruhr-University Bochum, Bürkle-de-la-Camp-Platz 1, 44789 Bochum, Germany*

MP 369 **Imaging Mass Spectrometry Reveals Spatially-Resolved Biomolecular Response to Heavy Metal Intoxication**; Emilio S Rivera[1, 2]; Kes A. Luchini[1, 2]; Tara Harvey[1, 2]; Madison Grace Thornhill[1, 2]; Robert M. Taylor[3]; Abdul-Mehdi S. Ali[3]; Alicia M. Bolt[4]; Srini R. Gadam[3]; Abigale S Mikolitis[1, 2]; Zachary J. Sasiene[1, 2]; Joshua D. Breidenbach[1, 2]; Ethan M. McBride[1, 2]; Brett R. Blackwell[1, 2]; Austin R. Anderson[1, 2]; Lauren K. Heine[1, 2]; Chi-Yen Tseng[1, 2]; Jessica A. Salguero[1, 2]; Francisca E. Rodriguez[1, 2]; Salvator J. Palmisano[1, 2]; Erick S. LeBrun[1, 2]; Phillip M. Mach[1, 2]; Justin T. Baca[3]; Trevor G. Glaros[1, 2]; *[1]Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [2]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [3]Department of Emergency Medicine, University of New Mexico School of Medicine, Albuquerque, NM; [4]Department of Pharmaceutical Sciences, College of Pharmacy, University of New Mexico, Albuquerque, NM*

MP 370 **Spatially resolved single-cell multi-omics via integration of metabolome and proteome profiling with mass spectrometry imaging**; Hua Zhang[1]; Xudong Shi[2]; Kelly H. Lu[3]; Zicong Wang[1]; Haiyan Lu[1]; Yuan Liu[1]; Nathan V. Welham[2]; Lingjun Li[1, 3]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of Surgery, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

MP 371 **Unveiling Spatial Metabolism in Mammalian Organ tissues: A Knowledge Base with Multimodal approach**; Prasad Phapale[1]; Siva Swapna Kasarla[1]; Karl Smith[1]; Antonia Fecke[1]; *[1]Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., Dortmund, Germany*

MP 372 **In-Depth Mapping of Antibodies and the Proteome by A New Generation of Micro-Scaffold-Assisted Proteomics (MASP) with Higher Spatial Resolution**; Shihan Huo[1]; Min Ma[1]; Shuo Qian[1]; Ming Zhang[1]; Jie Pu[1]; Xiaoyu Zhu[1]; Sailee Rasam[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY*

MP 373 **Quantitatively Mapping Thousands of Phosphorylated Proteins at the Whole Tissue Level by Micro-Scaffold-Assisted Spatial Phosphoproteomics (MASPhos)**; Min Ma[1]; Shihan Huo[1]; Ming Zhang[1]; Shuo Qian[1]; Maosheng Wei[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY*

MP 374 **Spatial Metabolomics and Isotope Tracing Reveal Division of Labor in the Mammalian Liver and Intestine**; Laith Samarah[1]; Xi Xing[1]; Clover Zheng[1]; Amichay Afriat[1]; Cong Ma[1]; Michael MacArthur[1]; Connor Jankowski[1]; Benjamin J. Raphael[1]; Joshua D. Rabinowitz[1]; *[1]Princeton University, Princeton, NJ*

MP 375 **Revealing the Molecular Underpinnings of Islet Dysfunction with Integrated Imaging Mass Spectrometry and Spatial Transcriptomics**; Angela R. S. Kruse[1]; Kristie I. Aamodt[2]; Chunhua Dai[3]; Morad C Malek[4, 5]; Roy Lardenoije[6]; Lukasz Migas[7]; Melissa A. Farrow[4, 5]; Diane Saunders[3]; Richard M. Caprioli[4, 8, 9]; Raf Van De Plas[7, 10]; Joana P. Gonçalves[6]; Alvin C. Powers[2, 3, 11]; Jeffrey M Spraggins[4, 5, 8, 9, 12]; *[1]Vanderbilt University, Nashville, TN; [2]Department of Molecular Physiology and Biophysics, Vanderbilt University School of Medicine, Nashville, TN; [3]Division of Diabetes, Endocrinology and Metabolism, Vanderbilt University Medical Center, Nashville, TN; [4]Mass Spectrometry Research Center, Nashville, TN; [5]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [6]Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands; [7]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [8]Department of Biochemistry, Vanderbilt University, Nashville, TN; [9]Department of Chemistry, Vanderbilt University, Nashville, TN; [10]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [11]Veteran Affairs Tennessee Valley Healthcare System, Nashville, TN; [12]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN*

MP 376 **Single-voxel proteomics for 2D-proteome mapping human spleen and mouse brain tissues**; Zhangyang Xu[1]; Reta Birhanu Kitata[1]; Rosalie K. Chu[2]; Rui Zhao[2]; Daniel J. Orton[2]; Thomas L. Fillmore[2]; Matthew J. Gaffrey[1]; Tong Zhang[1]; Tao Liu[1]; Clive H. Wasserfall[3]; Song-Lin Ding[4]; Tujin Shi[1]; *[1]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington; [2]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; [3]Department of Pathology, Immunology, and Laboratory Medicine, Diabetes Institute, College of Medicine, University of Florida, Gainesville, Florida; [4]Allen Institute for Brain Science, Seattle, Washington*

MP 377 **Preserving RNA integrity after Imaging Mass Spectrometry for Integrated Spatial Transcriptomics on Single Tissue Sections**; Morad C Malek[1, 2]; Martin Dufresne[1, 3]; Roy Lardenoije[4]; Angela RS Kruse[2, 5]; Lukasz Migas[1, 6]; Melissa A. Farrow[1, 3]; Katerina V Djambazova[1, 2]; Raf Van De Plas[1, 3, 6]; Joana P Gonçalves[4]; Jeffrey M Spraggins[1, 2, 3, 7, 8]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands; [5]Mass Spectrometry Research Center, Nashville, TN; [6]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [7]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; [8]Department of Chemistry, Vanderbilt University, Nashville, TN*

MP 378 **Laser Ablation Sampling and MALDI Imaging for Tissue Lipidomics**; Kadeem O Hayes[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

MP 379 **Constructing a Foundational Molecular Atlas of the Normal Human Kidney with Multimodal Molecular Imaging**; Olof Gerdur Isberg[1, 2]; Lukasz Migas[3]; Melissa A. Farrow[1, 4, 5]; Jamie L. Allen[1, 4]; Felipe A. Moser[3]; Léonore E.M. Tideman[3]; Angela R. S. Kruse[1, 2]; Ellie L. Pingry[1, 2]; Morad C. Malek[1]; Thai H. Pham[1, 2]; Madeline E. Colley[1, 4]; Haichun Yang[5, 6]; Mark P. DeCaestecker[2, 7]; Agnes B. Fogo[5, 6, 7]; Joana Goncalves[8]; Raf Van De Plas[3]; Jeffrey M. Spraggins[1, 2, 4, 5]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [3]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN; [5]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; [6]Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; [7]Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; [8]Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands*

MP 380 **Organoid analysis using ultra-high lateral resolution AP-SMALDI mass spectrometry imaging**; Parviz Ghezellou[1]; Elisa Badin[1]; Max A. Müller[1, 2]; Svenja Pauer[1]; Jasmin Ballout[1]; Vinicius Pinho Dos Reis[3]; Eva Hecker[3]; Martin Diener[1]; Kerstin Strupat[4]; Bernhard Spengler[1]; *[1]Justus Liebig University, Giessen, Germany; [2]Transmit GmbH, Giessen, Germany; [3]Philipps University, Marburg, Germany; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 381 **Single cell multi-omic mass spectrometry imaging for the human bone marrow microenvironment**; Patricia Favaro[1]; Davide Franchina[1]; Ke Xuan Leow[1]; Daniel Ho[1]; Trevor Bruce[1]; Xiaowei Lu[1]; Marc Bosse[1]; Richard R Drake[2]; Albert Tsai[1]; Michael Angelo[1]; Sean Bendall[1]; *[1]Stanford University, Stanford, CA; [2]Medical University of South Carolina, Charleston, SC*

MP 382 **SPOT: Spatial Proteomics through On-site Tissue-protein-labeling**; Yuanwei Xu[1, 2]; T.Mamie Lih[2]; Angelo Michael De Marzo[2, 3]; Qing Kay Li[3, 4]; Hui Zhang[1, 2, 3]; *[1]Johns Hopkins University, Baltimore; [2]Johns Hopkins University School of Medicine, Baltimore city, MD; [3]Johns Hopkins Sidney Kimmel Comprehensive Cancer Center, Baltimore, MD; [4]Johns Hopkins University School of Medicine, Baltimore, MD*

MP 383 **Delineating AβPlaque Associated Lipid Co-Aggregation Dynamics Using Pulse-Chase Spatial Multiomics**; Junyue Ge[1]; Durga Jha[1]; Srinivas Koutarapu[1]; Maciej Dulewicz[1]; Henrik Zetterberg[1, 2, 3, 4, 5]; Kaj Blennow[1, 2]; Jörg Hanrieder[1, 2, 3]; *[1]University of Gothenburg, Gothenburg, Sweden; [2]Sahlgrenska University Hospital, Gothenburg, Sweden; [3]University College London, London, United Kingdom; [4]Hong Kong Center for Neurodegenerative Diseases, Hong Kong, China; [5]University of Wisconsin-Madison, Madison, WI*

MP 384 **Rapid QCL-based Mid-Infrared Vibrational Microscopy guides Deep Magnetic Resonance MALDI MSI**; Stefan Schmidt[1]; Lars Gruber[2, 3]; Thomas Enzlein[2]; Huong Giang Vo[4]; James Lucas Cairns[2]; Denis Abu Sammour[2]; Matthias Eckhardt[5]; Laura Bindila[4]; Carsten Hopf[2, 3]; *[1]Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), University of Applied Sciences Mannheim, Mannheim, Germany; [2]Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), University of Applied Sciences Mannheim, Mannheim, Germany; [3]Medical Faculty, Heidelberg University, Heidelberg, Germany; [4]Clinical Lipidomics Unit, Institute of Physiological Chemistry, University of Medical Center of the JGU Uni Mainz, Mainz, Germany; [5]Institute of Biochemistry and Molecular Biology, University of Bonn, Bonn, Germany, Bonn, Germany*

INDUSTRY: TRACE ANALYSIS, QUALITY CONTROL, AND AUTOMATION

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MP 385 **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 386 **Trace-Level Quantification of N-Nitrosomethylpropylamine Impurity by LC-HRMS**; Ziyu Wang[1]; Holly M. Shackman[1]; Sloan Ayers[1]; Michael B. Peddicord[1]; Scott A. Miller[1]; *[1]Bristol Myers Squibb, New Brunswick, NJ*

MP 387 **Automated Sample Preparation using PAL3 RTC System for EPA 8270E Semi-volatile Organic Analysis by GC/TQ**; Tarun Anumol[1]; Gwen Sin Yee Lim[2]; Aimei Zou[3]; *[1]Agilent Technologies, Wilmington, DE; [2]CTC Analytics AG, Zwingen, Switzerland; [3]Agilent Technologies Singapore, Singapore, Singapore*

MP 388 **Automated Sample Preparation and Analysis of Organochlorine Pesticides (OCP’s) s in Drinking Water**; Callum Morgan[1]; Bryan White[2]; Joel Ferrer[3]; Aaron Boice[3]; Anastasia Andrianova[4]; *[1]Agilent Technologies UK Limited, Cheadle, United Kingdom; [2]Agilent Technologies LDA UK Ltd, Didcot, United Kingdom; [3]Agilent Technologies, Santa Clara, CA; [4]Agilent Technologies, Wilmington, DE*

MP 389 **Implementation of a digital quality management system for enhanced mass spectrometry practices in a large-scale proteomics laboratory**; Casey W Coutelin Johnson[1]; Shruti Rao[1]; Salomen Ashaq[1]; Susan M. Mockus[1]; *[1]Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA*

MP 390 **High resolution process gas monitoring by infiTOF to shed light on the growth process of β-Ga2O3 by MOVPE**; Yoshihiko Takinami[1]; Kazutaka Ikenaga[2]; Takahito Okuyama[3]; Shogo Sasaki[3]; Masato Ishikawa[4]; Yoshinao Kumagai[3]; *[1]Kanomax Analytical, Incorporated, Chofu, Japan; [2]Taiyo Nippon Sanso Corporation, Minato-ku, Japan; [3]Tokyo University of Agriculture and Technology, Koganei-shi, Japan; [4]Gas-Phase Growth Ltd., Koganei-shi, Japan*

MP 391 **Automated sample preparation instrument for large-scale proteomics pre-processing**; Lin He[1]; Yan Zhao[1]; Wei Sun[1]; Longqin Sun[1]; *[1]Beijing Qinglian Biotech Co., Ltd, Beijing, China*

MP 392 **Developing a Contaminant Spot Check and Removal Assay (ContamSPOT) for Mass Spectrometry Analysis**; Noah Smeriglio[1]; Haorong Li[1]; Wan Nur Atiqah Binti Mazli[1]; Katharine Bendel[1]; Ling Hao[1]; *[1]George Washington University, Washington D.C., DC*

MP 393 **High-speed compound quality assessment using Acoustic Ejection Mass Spectrometry**; Anuja Bhalkikar[1]; Aaron Stella[2]; Jacob Watson McCabe[2]; Han Joo Lee[2]; *[1]Sciex, Framingham; [2]SCIEX, USA, Framingham, MASSACHUSETTS*

MP 394 **Stability Testing of Consumer Drug Products for Benzene in Real-Time using SIFT-MS**; David Light[1]; Nicola Zenzola[1]; Amber Hudspeth[1]; Mara Dubnicka[1]; Kaury Kucera[1]; Wolfgang Hinz[1]; Christopher Bunick[2]; Arash Dabestani[3]; Leslie P. Silva[4]; *[1]Valisure, LLC, New Haven, CT; [2]Yale University, West Haven, CT; [3]Long Island University, Brooklyn, NY; [4]Syft Techologies, Anaheim, CA*

INFORMATICS: METABOLOMICS AND LIPIDOMICS

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MP 395 **Prioritizing Biotransformations in LC-MS/MS-based non-targeted Metabolomics with ChemProp2**; Abzer K Pakkir Shah[1]; Paolo Stincone[1, 2]; Anne Grießhammer[1, 3]; Axel Walter[1, 4]; Simon B Knoblauch[2]; Giovanni Andrea Vitale[1]; Mingxun Wang[5]; Lisa Maier[1, 3]; Daniel Petras[1, 6]; *[1]University of Tuebingen, CMFI Cluster of Excellence, Interfaculty Institute of Microbiology and Infection Medicine, Tübingen, Germany; [2]University of Tuebingen, Center for Plant Molecular Biology, Tübingen, Germany; [3]Cluster of*

Excellence EXC 2124 Controlling Microbes to Fight Infections, University of Tübingen, Tübingen, Germany; [4]Applied Bioinformatics, Department of Computer Science, University of Tübingen, Tübingen, Germany; [5]University of California Riverside, Department of Computer Science, Riverside, CA; [6]University of California Riverside, Department of Biochemistry, Riverside, CA

MP 396 **Metabolomics: Mapping Evolution and Trends in the Field with AI Tools**; Olatomiwa O Bifarin[1]; Varun S Yelluru[2]; Facundo M. Fernandez[1, 3]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Altanta, GA; [2]School of Computer Science, Georgia Institute of Technology, Atlanta, GA; [3]Petit Institute of Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA*

MP 397 **MyCompoundID 2.0: An Evidence-Based Metabolome Library for Metabolite Identification**; Bowen Yang[1]; Hao Li[1]; Shuang Zhao[2]; Liang Li[1, 2]; *[1]University of Alberta, Edmonton, AB; [2]The Metabolomics Innovation Centre (TMIC), Edmonton, AB*

MP 398 **Fiora: Learning fragmentation patterns of small compounds with graph neural networks** ; Yannek Nowatzky[1]; Thilo Muth[2]; Philipp Benner[1]; *[1]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany; [2]Robert Koch Institute, Berlin, Germany*

MP 399 **Big-data metabolomics: annotating MS/MS spectra for structures and biological relevance by querying extremely large scale datasets**; Yuanyue Li[1]; Oliver Fiehn[1]; *[1]UC Davis, Davis, CA*

MP 400 **Unmasking lipid double bond positions in routine LC-MS/MS data**; Leonida M Lamp[1]; Joseph P Argus[2]; Aaron M Armando[2]; Gosia M Murawska[2]; Oswald Quehenberger[2]; Edward A Dennis[2]; Jürgen Hartler[1, 3]; *[1]Pharmaceutical Sciences, University of Graz, Graz, Austria; [2]Department of Pharmacology, University of California San Diego, La Jolla, CA; [3]Field of Excellence BioHealth, University of Graz, Graz, Austria*

MP 401 **AI-driven peak picking and integration using chromatograms and deep neural networks**; Daniel Pelisek[1]; Radu Talmazan[1]; Martin Buratti[1]; Tuan Hai Pham[1]; Alice Limonciel[1]; *[1]biocrates life sciences ag – Eduard-Bodem-Gasse 8, Innsbruck, Austria*

MP 402 **Enhanced Structural Modification Site Localization through MS/MS Spectral Alignment and Molecular Network Refinement**; Mohammad Reza Zare Shahneh[1]; Michael Strobel[1]; Giovanni Andrea Vitale[2]; Christian Geibel[2]; Vanessa V Phelan[3]; Daniel Petras[4]; Allegra T Aron[5]; Yasin El Abiead[6]; Neha Garg[7]; Mingxun Wang[1]; *[1]University of California Riverside, Department of Computer Science, Riverside, CA; [2]University of Tuebingen, Interfaculty Institute of Microbiology and Infection Medicine, Tuebingen, Germany; [3]University of Colorado, Anschutz Medical Campus, Department of Pharmaceutical Sciences, Aurora, CO; [4]University of California Riverside, Department of Biochemistry, Riverside, CA; [5]University of Denver, Denver, CO; [6]University of California San Diego, La Jolla, CA; [7]Georgia Institute of Technology, Atlanta, GA*

MP 403 **TIMS-enabled 4D-Metabolomics workflow for the automated analysis of derivatised analytes**; Jesper Havelund[1]; Aiko Barsch[2]; Sofie Weinkouff[2]; Nikolas Kessler[2]; Heiko Neuweger[2]; Matthew R Lewis[2]; Nils J. Færgeman[1]; Ryo Nakabayashi[3]; *[1]Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark; [2]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; [3]Bruker Japan K.K., Yokohama, Japan*

MP 404 **Mapping of electron impact ionization time-of-flight and chemical ionization Fourier transform gas chromatographic mass spectrometry data by Genedata Expressionist**; Josh Prybil[1]; Joseph P. Shambaugh[2]; John D. Everard[1]; Brian M. Ruddy[1]; *[1]Corteva Agriscience, Johnston, IA; [2]Genedata Inc., Lexington, Massachusetts*

MP 405 **Automated LC-MS/MS Glycomic Structural Feature Annotation**; Xavier A. Holmes[1]; Armin Oulomi[1]; Michael Russelle S. Alvarez[1]; Ryan Schindler[1]; Tristan Seales[1]; Carlito B. Lebrilla[1]; *[1]University of California Davis, Davis, CA*

MP 406 **Utilizing Skyline in Automated System Suitability Testing, Data QC, and Metabolite Quantification for Microchip CE-MS Analysis**; Sam Stewart[1]; Erin A. Redman[2]; Joshua P. Guerrette[2]; Nicholas Shulman[3]; Brian S Pratt[3]; Michael J. MacCoss[3]; Brendan MacLean[3]; J. Will Thompson[2]; *[1]908 Devices Inc., Boston, MA; [2]908 Devices Inc, Morrisville, NC; [3]University of Washington - Genome Sciences, Seattle, WA*

MP 407 **PAMDA: Publicly Available Metabolomics Dataset Alignment and Analysis of Human Urine Measured by RPLC-MS**; Hani Habra[1]; Yamil Simon[1]; Tytus Mak[1]; *[1]NIST, Gaitherburg, MD*

MP 408 **LipidTarget: An Integrated Platform for Targeted HPLC-MSn Characterization and Quantification of Lipid sn-Positional Isomers**; Hongyuan Yang[1]; Tingyuan Yang[1]; Jiaxin Feng[1]; Xin Yan[1]; *[1]Texas A&M University, College Station, TX*

MP 409 **Metabolite-specific inter-individual variability: A meta-analysis of metabolomics datasets and the need for log transformation**; Aviral Singh[1]; Renu Pandey[2]; Gauri Desai[2]; Prajval Nakarni[1]; Vivek Mishra[1]; Deepti Sahasrabuddhe[2]; Pramod Wangikar[1, 2]; *[1]Clarity Bio Systems India Pvt. Ltd., Pune, India; [2]Indian Institute of Technology Bombay, Mumbai, India*

MP 410 **Comprehensive structural annotation of polar metabolites in human plasma using unified-HILIC/AEX retention time prediction and HRMS/MS substructure information**; Taihei Torigoe[1]; Masatomo Takahashi[1]; Omidreza Heravizadeh[2]; Kazuki Ikeda[1]; Kohta Nakatani[1]; Takeshi Bamba[1]; Yoshihiro Izumi[1]; *[1]Medical Institute of Bioregulation, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka-shi, Japan; [2]Graduate School of Systems Life Sciences, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka-shi, Japan*

MP 411 **LipiDex 2 integrates MSn tree-based fragmentation methods and quality control modules to improve discovery lipidomics**; Benton J. Anderson[1, 2]; Dain R. Brademan[3]; Yuchen He[4]; Corinne E. Moss[1]; Katherine A. Overmyer[1, 2, 3]; Gwendalyn J. Randolph[5]; Joshua J. Coon[1, 2, 3, 6]; *[1]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [2]National Center for Quantitative Biology of Complex Systems, Madison, WI; [3]Morgridge Institute for Research, Madison, WI; [4]Department of Biophysics, University of Wisconsin-Madison, Madison, WI; [5]Department of Pathology and Immunology, Washington University School of Medicine, St. Louis, MO; [6]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

MP 412 **Enhanced Spectrum Clustering For Increased Interpretability of Molecular Networking**; Janne Heirman[1]; Wout Bittremieux[1]; *[1]University of Antwerp, Antwerpen, Belgium*

MP 413 **Chemical Annotation Propagation for Molecular Networks**; Bela Paizs[1, 2]; Logan Mackay[1]; Amar Rai[3]; Anthony J Devlin[1]; Zoltan Takats[2, 3]; *[1]Rosalind Franklin Institute, Didcot, United Kingdom; [2]deShape ltd., London, United Kingdom; [3]Imperial College London, London, United Kingdom*

MP 414 **MS2LIPID: lipid subclass prediction using tandem mass spectral data**; Nami Sakamoto[1]; Takaki Oka[1]; Yuki Matsuzawa[1]; Kozo Nishida[1]; Aya Hori[2]; Makoto Arita[2, 3, 4]; Hiroshi Tsugawa[1, 2, 4, 5, 6]; *[1]Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology, Koganei-shi, Japan; [2]Laboratory for Metabolomics, RIKEN Center for Integrative Medical Sciences, Yokohama, Japan; [3]Keio University, Graduate School of Pharmaceutical Sciences, Division of Physiological Chemistry and Metabolism,, Minato-ku, Japan; [4]Molecular and Cellular Epigenetics Laboratory, Graduate School of*

Medical Life Science, Yokohama City University, Yokohama, Japan; [5]RIKEN Center for Brain Science, Wako, Japan; [6]RIKEN Center for Sustainable Resource Science, Yokohama, Japan

MP 415 **Deep Learning for Small Molecule Analog Discovery From Untargeted Mass Spectrometry**; Juan Sebastian Piedrahita Giraldo[1]; Thomas De Vijlder[2]; Kris Laukens[1]; Wout Bittremieux[1]; *[1]University of Antwerp, Antwerp, Belgium; [2]Janssen Pharmaceutica NV, Beerse, Belgium*

MP 416 **Evaluation of an R-based metabolomics data processing workflow against a novel benchmark metabolomics dataset**; Corey D Broeckling[1]; Linxing Yao[1]; Nathan Montgomery[1]; Kevin Y Cho[2]; Gary J. Patti[2]; Xiuxia Du[3]; *[1]Colorado State University, Fort Collins, CO; [2]Washington University in Saint Louis, St. Louis, MO; [3]University of North Carolina at Charlotte, Charlotte, NC*

MP 417 **Deciphering the Interplay between 16S rRNA-seq and Metabolome through Weighted Correlation Network Analysis**; Minsoo Son[1]; Jong Hee Song[1]; Young Ah Goo[1]; *[1]MTAC, MGI, Washington University School of Medicine in Saint Louis, Saint Louis, MO*

MP 418 **Reanalysis of public domain, untargeted metabolomics datasets using AI-powered workflow: Unraveling novel biomarkers for severe COVID**; Prajval Nakrani[1]; Nived Krishnan Santhosh[1]; Aviral Singh[1]; Vivek Mishra[1]; Sachin Patil[1]; Pramod P Wangikar[1, 2]; *[1]Clarity Bio Systems India Pvt. Ltd., Pune, India; [2]Indian Institute of Technology Bombay, Mumbai, India*

MP 419 **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[1]; Ian Morns[1]; Pete Reay[1]; Simon Jones[1]; Nyasha Munjoma[1]; Jayne Kirk[1]; Richard Lock[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

MP 420 **Extensive multi language API-support and novel annotation features in SIRIUS**; Markus Fleischauer[1]; Kai Dührkop[1]; Martin A. Hoffmann[2]; Marcus Ludwig[2]; Nils A. Haupt[1]; Martin Engler-Lukajewski[2]; Jonas Emmert[1, 3]; Michael Stravs[4]; Sebastian Böcker[1]; *[1]Friedrich Schiller University Jena, Jena, Germany; [2]Bright Giant GmbH, Jena, Germany; [3]International Max Planck Research School "Chemical Communication in Ecological Systems", Max Planck Institute for Chemical Ecology, Jena, Germany; [4]Eawag (Swiss Federal Institute of Aquatic Science and Technology) / Environmental Microbiology, Dübendorf, Switzerland*

MP 421 **Rapid and Precise Small Molecule Detection in Untargeted Metabolomics Using MetaboSLASH**; Sujun Li[1, 2]; Haixu Tang[1]; *[1]Indiana University, Bloomington, IN; [2]GlycoMS LLC, Bloomington, IN*

MP 422 **Isocitrate dehydrogenase 1 regulates cardiac metabolic adaptation during oncometabolic stress**; Kyoungmin Kim[1]; Brandon Faubert[2]; Yaqi Gao[1]; Lin Tan[3]; Nathaniel Snyder[4]; Philip L. Lorenzi[5]; Ralph DeBerardinis[6]; Anja Karlstaedt[1]; *[1]Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA; [2]University of Chicago, Chicago, IL; [3]MD Anderson Cancer Center, Houston, Texas; [4]Temple University, Philadelphia, PA; [5]MD Anderson Cancer Center, Houston, TX; [6]UTSouthwestern Medical Center, Dallas, TX*

MP 423 **Learned representations from a transformer model trained on over 1 billion unannotated experimental spectra**; James Taylor[1]; Rose Lightheart[1]; Christoph Krettler[1]; Tyson Park[1]; Daniel Domingo-Fernandez[1]; David Healey[1]; *[1]Enveda Biosciences, Boulder, CO*

MP 424 **Fast and Precise Hybrid Gas-Chromatography Mass-Spectrometry Metabolomics, Combining Single-Sample Targetted Search with Untargetted Composite Feature Detection**; Sami Teeny[1]; Dean P. Jones[2]; Young-Mi Go[2]; William Crandall[2]; Bill Liang[2]; Zackery Ryan Jarrell[2]; *[1]University, Atlanta, GA; [2]Emory University, Atlanta, GA*

MP 425 **Machine learning based filtering improves untargeted lipid identification confidence**; Steven Tavis[1, 2]; Matthew J. Keller[2, 3]; Andrew Stai[3]; Diana Ramirez[3]; Frank Loeffler[3]; Robert L Hettich[2]; *[1]University of Tennessee Knoxville, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]University of Tennessee, Knoxville, TN*

MP 426 **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[1]; Benjamin L. Oyler[1]; Constantinos Petrovas[1]; Richard Koup[1]; *[1]Tissue Analysis Core, Immunology Laboratory, Vaccine Research Center, NIAID, NIH, Bethesda, Maryland*

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MP 427 **Contrasting Trends: Increasing Variance at High Purity Levels in TMT Reporter Ion Analysis**; Eric Younggon Kim[1]; Dhonggeon Won[2]; Chaewon Kang[3]; Hokeun Kim[3]; Sang-Won Lee[3]; Sangtae Kim[1]; *[1]Bertis Bioscience, SAN DIEGO, CA; [2]Bertis Inc., Seoul, South Korea; [3]Department of Chemistry and Center for Proteogenome Research, Seoul, South Korea*

MP 428 **Phosphorylation site prediction model using structural context and its application to phosphopeptide identification**; Yujin Choo[1]; Seungjin Na[2]; Eunok Paek[3, 4, 5]; *[1]Department of Artificial Intelligence, Hanyang University, Seoul, South Korea; [2]Korea Basic Science Institute, Cheongju, South Korea; [3]Department of Artificial Intelligence, Hanyang University, Seoul, South Korea; [4]Department of Computer Science, Hanyang University, Seoul, South Korea; [5]Institute of Artificial Intelligence Research, Hanyang University, Seoul, South Korea*

MP 429 **EndoGenius – An All-in-One Platform for Comprehensive Neuropeptidome Characterization from DDA and DIA Datasets**; Lauren Fields[1]; Tina C Dang[2]; Mitchell Gray[1]; Wenxin Wu[1]; Angel E Ibarra[1]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin; [2]University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin*

MP 430 **Prosit-PTM: Deep Learning Model Enhances Detection and Localization of Unseen PTMs**; Wassim Gabriel[1]; Vitor Sternlicht[1]; Daniel P. Zolg[2]; Polina Prokofeva[2]; Ludwig Lautenbacher[1]; Guillaume Médard[2]; Chien-Yun Lee[3]; Bernhard Kuster[2]; Mathias Wilhelm[1]; *[1]Computational Mass Spectrometry, TUM, Freising, Germany; [2]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [3]Young Investigator Group: Mass Spectrometry in Systems Neurosciences, School of Life Sciences, Technical University of Munich, Freising, Germany*

MP 431 **ProteoBench: a community-curated platform for comparison of proteomics data analysis workflows**; Holda A Anagho[1]; Sven Degroeve[2, 3]; Nadezhda T Doncheva[1]; Viktoria Dorfer[4]; Klemens Fröhlich[5]; Ralf Gabriels[2, 3]; Vedran Kasalica[6]; Caroline Lennartsson[1]; Matthias Mattanovich[7]; Emmanuelle Mouton-Barbosa[8]; Martin Rykær[1]; Veit Schwämmle[9]; Maximilian T. Strauss[1]; Julian Uszkoreit[10]; Bart Van Puyvelde[11]; Tim Van Den Bossche[2, 3]; Jakub Vašíček[12, 13]; Henry Webel[7]; Witold Wolski[14, 15]; Robbin Bouwmeester[2, 3]; Marie Locard-Paulet[8]; *[1]Novo Nordisk Foundation Center for Protein Research (CPR), University of Copenhagen, Copenhagen, Denmark; [2]VIB-UGent Center for Medical Biotechnology, Gent, Belgium; [3]Department of Biomolecular Medicine, Ghent University, Gent, Belgium; [4]University of Applied Sciences Upper Austria, Hagenberg, Austria; [5]Proteomics Core Facility, Biozentrum Basel, University of Basel, Basel, Switzerland; [6]Netherlands eScience Center,, Amsterdam, Netherlands; [7]Novo Nordisk Foundation Center for Basic Metabolic Research, Copenhagen, Denmark; [8]Institut de Pharmacologie et de Biologie Structurale (IPBS), Université de Toulouse, CNRS, Université Toulouse III - Paul Sabatier (UT3), Toulouse, France, Toulouse, France; [9]Department of Biochemistry and Molecular Biology, University of Southern Denmark,, Odense, Denmark; [10]Ruhr University Bochum,* *Medical Faculty, Medical Bioinformatics, Bochum, Germany; [11]ProGenTomics, Laboratory of Pharmaceutical Biotechnology, Ghent University, Ghent, Belgium; [12]Mohn Center for Diabetes Precision Medicine, Department of Clinical Science, University of Bergen, Bergen, Norway; [13]Computational Biology Unit, Department of Informatics, University of Bergen, Bergen, Norway; [14]Functional Genomics Center Zurich – ETH Zurich/University of Zurich, Zurich, Switzerland; [15]Swiss Institute of Bioinformatics (SIB), Lausanne, Switzerland*

MP 432 **NeoFlow2: Enhancing Tumor-Specific HLA-I Peptide Identification by Integrating De Novo Sequencing and Customized Database Search in a Streamlined Proteogenomic Workflow**; Seunghyuk Choi[1]; Yongchao Dou[1]; Zhiao Shi[1]; Bing Zhang[1]; *[1]Baylor College of Medicine, Houston, TX*

MP 433 **Alternating series approximation minimizes quantitative bias arising from incomplete isotope labeling**; Pin-Lian Jiang[1]; Louise Ulrich Kurt[2]; Isis Venturi Biembengut[2]; Fan Liu[1]; *[1]Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; [2]Laboratory for Structural and Computational Proteomics, Fiocruz-Parana, Curitiba, Brazil*

MP 434 **Impact of the Peptide Identification Framework on the Results of Fast Photochemical Oxidation of Protein Analysis**; Marek Zakopcanik[1, 2]; Daniel Kavan[1]; Petr Novak[1]; Dmitry S. Loginov[1]; *[1]Institute of Microbiology, Praha - Vestec, Czech Republic; [2]Department of Biochemistry, Faculty of Science, Charles University, Prague 2, Czech Republic*

MP 435 **Optimized Clustering and Neighbor-Informed Re-identification of Spectra in a Spectral Archive by Complete Pair-wise Similarity Calculations and DBSCAN Clustering**; Ayman Hoque[1]; Henry Lam[1]; *[1]Hong Kong University of Science and Technology, HONG KONG, Hong Kong*

MP 436 **DeepCCS: Context-aware prediction of peptide collisional cross section increases peptide recovery for out-of-distribution data-independent acquisition (DIA) datasets**; George Rosenberger[1, 2]; Ignacio Jáuregui Novo[2, 3]; Alexandros Pachos[2]; An-phi Nguyen[2]; Tejas Gandhi[2]; Dennis Trede[4]; Lukas Reiter[2]; *[1]Bruker Switzerland AG, Faellanden, Switzerland; [2]Biognosys AG, Schlieren, Switzerland; [3]Mestrelab Research S.L., Santiago de Compostela, Spain; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

MP 437 **Toward Massively Pooled Screens of Covalent Ligands Using a New Multi-Modification Comet Search**; Kean Hean Ooi[1]; Jimmy Eng[2]; Ramin Rad[1]; Ka Yang[1]; Brandon Gassaway[3]; Steven Shuken[1]; Julian Mintseris[1]; Qing Yu[1]; Joao A. Paulo[1]; Edward L. Huttlin[1]; Steven P. Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Washington University in Saint Louis, St. Louis, MO; [3]Brigham Young University, Provo, UT*

MP 438 **DelPi: Genuine library-free peptide identification in DIA data through deep feature learning**; Jungkap Park[1]; Dhonggeon Won[1]; Dmitry Avtonomov[2]; Sangtae Kim[2]; *[1]Bertis Inc, Seoul, South Korea; [2]Bertis Bioscience, SAN DIEGO, CA*

MP 439 **Data-independent acquisition represents a promising alternative for FPOP samples analysis**; Marek Zakopcanik[1, 2]; Dmitry S. Loginov[1]; Daniel Kavan[1]; Petr Novak[1]; *[1]Institute of Microbiology of the Czech Academy of Sciences, 142 20, Prague, Czech Republic; [2]Department of Biochemistry, Charles University, Prague, Czech Republic*

MP 440 **Toward In-Depth MS1 Analysis of MS-Based Proteomics with PepPre2**; Ching Tarn[1]; Kai-Fei Wang[1]; Hao Chi[1]; *[1]Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China*

MP 441 **PiQuant: software for rapid and accurate quantification of mass spectrometry-based proteomics data**; Pedro Moreno Cardoso[1]; David N. Perkins[1]; Nazrath Nawaz[1]; Weronika S. Borek[1]; Josie A. Christopher[1]; Amy E. Campbell[1]; Andrew Williamson[1]; Pedro R. Cutillas[1, 2]; Arran D. Dokal[1]; *[1]Kinomica Ltd, Macclesfield, Cheshire, United Kingdom; [2]Barts Cancer Institute, Queen Mary University of London, London, United Kingdom*

MP 442 **Sunshine and rainbows: constructive interference and the deconvolution of peptide MS1 spectra**; Florian Seefried[1]; Alexander Hogrebe[1]; Patroklos Samaras[1]; Michael Graber[1]; Michelle T Berger[1]; Daniel P Zolg[1]; Mathias Wilhelm[2]; Martin Frejno[1]; *[1]MSAID, Garching, Germany; [2]Technical University of Munich, Computational Mass Spectrometry, Freising, Germany*

MP 443 **MS1-based feature generation to improve identification rate in single cell proteomics datasets**; Sam Van Puyenbroeck[1, 2]; Arthur Declercq[1, 2]; Tine Claeys[1, 2]; Ralf Gabriels[1, 2]; Lennart Martens[1, 2]; *[1]VIB - UGent Center for Medical Biotechnology, Gent, Belgium; [2]Department of Biomolecular Medicine, Ghent University, Ghent, Belgium*

MP 444 **Peptide ancestral-informative markers for inferring the proportion of ancestry**; Yurou Huang[1]; Keyue Ding[2]; Songfeng Wu[3]; Yunping Zhu[1]; *[1]State Key Laboratory of Medical Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences (Beijing), Beijing Institute of Lifeomics, Beijing, China; [2]Department of Cardiovascular Medicine, Mayo Clinic, Rochester, MN; [3]Beijing Qinglian Biotech Co., Ltd,, Beijing, China*

MP 445 **Big Data, Small Organisms: A holistic view on the community-wide assembled E. coli Proteome**; Caroline Jachmann[1, 2]; Aurélie Hirschler[3]; Florence Arsène-Ploetze[4]; Christine Carapito[3]; Luis Mendoza[5]; Eric W Deutsch[5]; Zhi Sun[5]; Ralf Gabriels[1, 2]; Robbin Bouwmeester[1, 2]; Kay Nieselt[6]; Tim Van Den Bossche[1, 2]; Lennart Martens[1, 2]; *[1]VIB-UGent Center for Medical Biotechnology, VIB, Ghent, Belgium; [2]Department of Biomolecular Medicine, Ghent University, Gent, Belgium; [3]BioOrganic Mass Spectrometry Laboratory (LSMBO), IPHC UMR 7178, University of Strasbourg, CNRS, ProFI, Strasbourg, France; [4]Institut de biologie moléculaire des plantes, CNRS, Université de Strasbourg, Strasbourg, France; [5]Institute for Systems Biology, Seattle, Washington; [6]Institute for Bioinformatics and Medical Informatics, University of Tübingen, Sand 14, 72076, Tübingen, Germany*

MP 446 **Pioneer: Fast and Open-Source Algorithms for Analyzing Data-Independent Acquisition Proteomics Experiments**; Nathan T Wamsley[1]; Michael B Major[1]; Dennis Goldfarb[1]; *[1]Washington University in Saint Louis, St. Louis, MO*

MP 447 **Oktoberfest: search engine agnostic rescoring pipeline leveraging online peptide property prediction from various models**; Mario Picciani[1, 2]; Wassim Gabriel[1]; Ludwig Lautenbacher[1]; Armin Soleymaniniya[1, 2]; Xiao Zixuan[1]; Eva Ayla Schroeder[1]; Matthew The[3]; Mostafa Kalhor[1]; Charlotte Adams[4]; Wout Bittremieux[4]; Kurt Boonen[5]; Mathias Wilhelm[1, 2]; *[1]Computational Mass Spectrometry, TUM, Freising, Germany; [2]Elite Network Bavaria, TUM, Freising, Germany; [3]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [4]Department of Computer Science, University of Antwerp, Antwerp, Belgium; [5]Department of Biomedical Sciences, University of Antwerp, Antwerp, Belgium*

MP 448 **tims2Rescore: A DDA-PASEF optimized data-driven identification rescoring pipeline**; Arthur Declercq[1, 2]; Robbe Devreese[1, 3]; Jonas Scheid[4, 5, 6]; Caroline Jachmann[1, 3]; David Gomez-Zepeda[7, 8, 9]; Jeewan Babu RIJAL[10]; Aurélie Hirschler[10]; Jonathan R Krieger[11]; Tharan Srikumar[11]; George Rosenberger[12]; Dennis Trede[13]; Christine Carapito[10]; Stefan Tenzer[7, 8, 14, 15]; Juliane Walz[4, 5, 16]; Sven Degroeve[1, 3]; Robbin Bouwmeester[1, 3]; Lennart Martens[1, 3]; Ralf Gabriels[1, 3]; *[1]VIB / UGent - Center for Medical Biotechnology (CMB), Gent, Belgium; [2]Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; [3]Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; [4]Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tübingen,*

Tübingen, Germany; [5]Cluster of Excellence iFIT (ECX2180) "Image-Guided and Functionally Instructed Tumor Therapies"; University of Tuebingen, Tuebingen, Germany; [6]Quantitative Biology Center (QBiC), University of Tübingen, Tübingen, Germany; [7]Institute of Immunology, University Medical Center of the Johannes-Gutenberg University, Mainz, Germany; [8]Helmholtz Institute for Translational Oncology Mainz (HI-TRON Mainz) – A Helmholtz Institute of the DKFZ, Mainz, Germany; [9]German Cancer Research Center (DKFZ) Heidelberg, Division 191 & Immunopeptidomics Platform, Heidelberg, Germany; [10]BioOrganic Mass Spectrometry Laboratory (LSMBO), IPHC UMR 7178, University of Strasbourg, CNRS, ProFI, Strasbourg, France; [11]Bruker Ltd., Milton, ON; [12]Bruker Switzerland AG, Faellanden, Switzerland; [13]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [14]German Cancer Research Center (DKFZ) Heidelberg, Division 191, Heidelberg, Germany; [15]Research Center for Immunotherapy (FZI), University Medical Center of the Johannes-Gutenberg University, Mainz, Germany; [16]Clinical Collaboration Unit Translational Immunology, Department of Internal Medicine, University Hospital Tuebingen, Tuebingen, Germany

MP 449 **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[1]; Tobias Schmidt[1]; Siegfried Gessulat[2]; Florian Seefried[1]; Michael Graber[1]; Samia Ben Fredj[1]; Patroklos Samaras[1]; Markus Schneider[1]; Layla Eljagh[1]; Vishal Sukumar[1]; Michelle T Berger[1]; Alexander Hogrebe[2]; Igor Bronshtein[2]; Pedro Navarro[3]; Kai Fritzemeier[3]; Yovany Cordero Hernandez[3]; Frank Berg[3]; Carmen Paschke[3]; David M Horn[4]; Philip L Loziuk[4]; Bernard Delanghe[3]; Christoph Henrich[3]; Martin Heinrich Frejno[1]; *[1]MSAID, Garching, Germany; [2]MSAID, Berlin, Germany; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Thermo Fisher Scientific, San Jose, CA*

MP 450 **FragPipe Advancements for Optimized DDA, DDA+, and DIA Mass Spectrometry Data Analysis**; Fengchao Yu[1]; Yamei Deng[1]; Daniel A. Polasky[1]; Kevin L. Yang[1]; Kai Li[1]; Guo Ci Teo[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, Michigan*

MP 451 **De novo sequencing of multiple peptides in chimeric mass spectra**; Yanik Bruns[1]; Mathias Wilhelm[2, 3]; Julien Gagneur[1, 3, 4, 5]; *[1]Computational Molecular Medicine, School of Computation, Information and Technology, Technical University of Munich, Munich, Germany; [2]Computational Mass Spectrometry, TU Munich, TUM School of Life Sciences, Freising, Germany; [3]Munich Data Science Institute, Technical University of Munich, Garching bei Muenchen, Germany; [4]Institute of Human Genetics, School of Medicine, Technical University of Munich, Munich, Germany; [5]Computational Health Center, Helmholtz Center Munich, Neuherberg, Germany*

MP 452 **Confident identification of proteome-wide low-level mutations using PEAKS 11.5**; Kyle Hoffman[1]; Julie Genereaux[2]; Lei Xin[1]; Zia Rahman[1]; Christopher J Brandl[2]; Patrick O'Donoghue[2]; Baozhen Shan[1]; *[1]Bioinformatics Solutions Inc., Waterloo, ON; [2]Western University, London, Ontario*

MP 453 **The Synergistic Effect of combining Prosit rescoring with SIMSI-Transfer for Clinical Cancer Cohorts**; Firas Hamood[1]; Pia Pfeiffer[1]; Wassim Gabriel[1]; Mathias Wilhelm[1]; Bernhard Kuster[1]; Matthew The[1]; *[1]Technical University of Munich (TUM), Freising, Germany*

MP 454 **Improving single-cell data interpretation by joint modeling of peptide fragmentation spectra**; Kevin McDonnell[1]; Harrison Specht[1]; Nikolai Slavov[1, 2]; *[1]Parallel Squared Technology Institute, Watertown, MA; [2]Northeastern University, Boston, MA*

MP 455 **Conceptual Framework for SCP Chimeric Spectra Annotation**; Alyssa A Nitz[1]; Samuel H Payne[1]; *[1]Brigham Young University, Provo, UT*

MP 456 **Fragment ion indexing accelerates Comet database search and expands real-time search capabilities**; Erik J Bergstrom[1]; Jimmy Eng[1]; Chris McGann[1]; Fengchao Yu[2]; Qing Yu[3]; Alexey I Nesvizhskii[2]; Devin K Schweppe[1]; *[1]University of Washington - Genome Sciences, Seattle, WA; [2]University of Michigan, Ann Arbor, MI; [3]Harvard Medical School, Boston, MA*

MP 457 **Integrative bioinformatic analysis of human lysine ubiquitylation provides insight into strategies for comprehensive site-localized ubiquitylomics**; Regina M. Edgington[1]; Damien B Wilburn[2]; *[1]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; [2]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio*

ION MOBILITY: APPLICATIONS I
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MP 458 **Flow injection analysis of isomers of new psychoactive substances using cyclic ion mobility mass spectrometry**; Marianna Nytka[1]; František Tureček[2]; Karel Lemr[1]; *[1]Department of Analytical Chemistry, Faculty of Science, Palacký University, Tr. 17. listopadu 12, 779 00, Olomouc, Czech Republic; [2]Department of Chemistry, University of Washington, Seattle, WA*

MP 459 **Implementation of native RapidFire ion mobility mass spectrometry (nRF-IM-MS) for assessment of the higher order structure (HOS) stability of biotherapeutics**; Mack Shih[1]; Patrick J Faustino[1]; Xiaoming Xu[1]; Jinhui Zhang[1]; *[1]Food and Drug Administration, Silver Spring, MD*

MP 460 **A Collision-Induced Dissociation-Trap Ion Mobility (CID-TIMS) Workflow for Site-Specific Identification of Isomerized Residues in Neuropeptides**; Samuel Okyem[1, 2]; Jonathan V Sweedler[1, 2]; *[1]university of Illinois-Urbana Champaign, Urbana, IL; [2]Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Champaign, IL*

MP 461 **Online radioligand therapy reaction monitoring optimization and chelation efficiency by cyclic ion mobility spectrometry-mass spectrometry**; Brooke Brown[1]; Samuel Annan[1]; Rohit Duvadie[1]; Richard Robinson[1]; *[1]Novartis Biomedical Research, cambridge, MA*

MP 462 **Exploring Ion Mobility Data File Conversions to Leverage Existing Tools and Enable New Workflows**; Sarah M. Stow[1]; Hannah Florance[1]; David A. Weil[1]; Bryson Gibbons[2]; Aivett Bilbao[2]; Richard Knochenmuss[3]; Ruwan T. Kurulugama[1]; John C. Fjeldsted[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]Pacific Northwest National Laboratory, Richland, WA; [3]RKResearch, Seftigen, Switzerland*

MP 463 **Enhancing Host Cell Protein (HCP) Analysis using SLIM-based Orbitrap Platform**; Liulin Deng[1]; Alan McKenzie-Coe[1]; Greg Kilby[1]; Kyle L. Fort[2]; Brian Adamson[3]; Oliver M Bernhardt[4]; Roland Bruderer[4]; Tejas Gandhi[4]; Lukas Reiter[4]; Eloy R. Wouters[3]; Jean-Jacques Dunyach[3]; Daniel DeBord[1]; Alexander A. Makarov[2]; *[1]MOBILion Systems, Chadds Ford, PA; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermo Fisher Scientific, San Jose, CA; [4]Biognosys AG, Schlieren, Switzerland*

MP 464 **Nucleotide derivative isomers analysis using ion mobility spectrometry and theoretical calculations**; Chuan-Fan Ding[1]; Fangling Wu[1]; *[1]Ningbo University, Ningbo, China*

MP 465 **An Ion Mobility Collision Cross Section Database in Support of the Periodic Table of Food Initiative**; Jody C May[1]; Katrina L Leaptrot[1]; Chi-Ming Chien[2]; Tracy Shafizadeh[2]; Steve Watkins[2]; Stacy D Sherrod[1]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]Verso Biosciences, Davis, CA*

MP 466 **Assessing selectivity of deubiquitinating enzymes via ion mobility-based analysis of polyubiquitin isomers**;

Elizaveta Shestoperova[1]; Eric R Strieter[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

MP 467 **The Utility of Cyclic Ion Mobility to Improve Selectivity and Analysis Efficiency of Environmental PFAS Contamination and Exposure**; Michael McCullagh[1]; Iggy Kass[2]; Georgios Theodoridis, [3]; Artemis Lioupi[3]; Robert Plumb[2]; Sarah Dowd[4]; Stuart Adams[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]Laboratory of Analytical Chemistry, School of Chemistry, Aristotle University of Thessaloniki, Thermi, Greece; [4]Waters, Milford, MA*

MP 468 **Characterization using ion mobility MS and energy minimization modeling of conformational distinctions between mono- and diphosphorylated PIPs**; Hernando Olivos[1]; Prithviraj Nandigrami[2]; Steven Lai[1]; Christopher Jurtschenko[1]; Yunping Qiu[2]; Andras Fiser[2]; Irwin J. Kurland[2]; *[1]Waters Corporation, Milford, MA; [2]Albert Einstein College of Medicine, Bronx, NY*

MP 469 **In-depth investigation of PFAS occurrence in environmental samples combining LC-VIP HESI-TIMS-QTOF MS with PASEF and untargeted data processing**; Georgios Gkotsis[1]; Dimitrios E. Damalas1[1]; Bob Galvin[2]; Carsten Baessmann[3]; Nikolaos S. Thomaidis[1]; *[1]National and Kapodistrian University of Athens, Department of Chemistry, Laboratory of Analytical Chemistry, Athens, Greece; [2]Bruker Daltonics, Coventry, United Kingdom; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

MP 470 **Structural Characterization of Endogenous Endocrine Hormone Isomers usingHigh-Resolution SLIM Ion Mobility**; Makenna K Hoover[1]; Christopher D. Chouinard[1]; *[1]Clemson University, Clemson, SC*

MP 471 **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 472 **Characterization of Microcystin Compounds Using High Resolution Ion Mobility Mass Spectrometry**; Esabella R Powers[1]; Jae Hwan Lee[1, 2]; Michael W Christopher[1]; Krista McCoy[3]; Daniel DeBord[4]; Sarah M. Stow[5]; Ruwan T Kurulugama[5]; Boone M. Prentice[1]; Richard A Yost[1]; Timothy J. Garrett[1, 6]; *[1]Department of Chemistry, University of Florida, Gainesville, FL; [2]Air Force Institute of Technology, United States Air Force, Wright-Patterson AFB, OH; [3]Harbor Branch Oceanographic Institute, Florida Atlantic University, Fort Pierce, FL; [4]MOBILion Systems, Inc., Chadds Ford, PA; [5]Agilent Technologies, Santa Clara, CA; [6]Department of Pathology, Immunology and Laboratory Medicine and Southeast Center for Integrated Metabolomics, University of Florida, Gainesville, FL*

MP 473 **Collision Cross Section Prediction using Graph Neural Networks for improved compound identification**; Shaurya Chanana[1]; Chloe Engler Hart[1]; António José Preto[1]; Daniel Domingo-Fernandez[1]; Tobias Kind[1]; David Healey[1]; *[1]Enveda Biosciences, Boulder, CO*

MP 474 **Enabling Protein and Oligonucleotide Ion Mobility Data Analysis in BioConfirm with PNNL Preprocessor Data Conversions**; Gordon W. Slysz[1]; Sarah M. Stow[2]; Jack P. Ryan[3]; Erin S. Baker[3]; Rebecca Glaskin[2]; Michael D. Knierman[2]; Aivett Bilbao[4]; Bryson Gibbons[4]; Christian Klein[2]; Ruwan T. Kurulugama[2]; Crystal Cody[2]; John C. Fjeldsted[2]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies, Santa Clara, CA; [3]University North Carolina at Chapel Hill, Chapel Hill, NC; [4]Pacific Northwest National Laboratory, Richland, WA*

MP 475 **Analysis of Gas Phase Protein Complex Unfolding in Positive and Negative nESI**; Martha Ortega Zepeda[1, 2]; Yu-Fu Lin[1, 2]; Dalton T Snyder[2]; Vicki H Wysocki[1, 2]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH*

MP 476 **Separation of Isobaric Amino acids and Small Molecule Metabolites Using Multipass Ion Mobility Analysis**; Hernando Olivos[1]; Jorge Smith[1]; Eve L Berger[2]; *[1]Waters Corporation, Milford, MA; [2]National Aeronautics and Space Administration, Houston, TX*

MP 477 **Ride the Wave: Challenging Enantiomeric separation Using SLIM-Ion Mobility Mass Spectrometry**; Meenakshi Goel[1]; Sayyeda Zeenat A Razvi[1]; Jose G Napolitano[2]; Sreya Sarkar[2]; Christopher M Crittenden[2]; *[1]Genentech Inc., South San Francisco, CA; [2]Genentech Inc, South San Francisco, CA*

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MP 478 **Aza-Prilezhaev Aziridination-Enabled Multidimensional Analysis of Isomeric Lipids via High-Resolution U-Shaped Mobility Analyzer-Mass Spectrometry**; Yuling Li[1]; Yiming Wang[1]; Kang Guo[1]; Kuofeng Tseng[1]; Xiaoqiang Zhang[1]; Wenjian Sun[1]; *[1]Shimadzu Research Laboratory (Shanghai) Co. Ltd., Shanghai, China*

MP 479 **Isomer-resolving CE-MS enables comprehensive analysis of lipidome in single cell spheroids**; Wenpeng Zhang[1]; Junhan Wu[2]; Yikun Liu[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China; [2]PURSPEC Technology (China) Ltd., Suzhou, China*

MP 480 **Identification of Double Bond Positions in Ceramides from the Stratum Corneum Using OAD-TOF System**; Yohei Arao[1]; Mami Okamoto[1]; Hidenori Takahashi[1]; *[1]Shimadzu Corporation, Nakagyo-ku, Japan*

MP 481 **Structural Elucidation of Copper-complexed Phosphatidylcholines via Tandem Mass Spectrometry**; Zunaira Naeem[1]; Tingting Yan[2]; Julia R. Bonney[2]; Boone M. Prentice[2]; *[1]University of Florida, Gainesville, FL; [2]University of Florida, GAINESVILLE, FL*

MP 482 **Characterization of Lipid Isomers Observed During Lipidomic LX-MS via Ozone-Induced Dissociation Mass Spectrometry (OzID-MS)**; Kimber N. Focke[1]; James D. Sanders[1]; Michael T. Marty[1]; *[1]University of Arizona, Tucson, AZ*

MP 483 **Data independent acquisition coupled with electron activated dissociation for hydroxy position resolved profiling of FAHFA**; Yuto Kurizaki[1]; Yuki Matsuzawa[1]; Kanako Tokiyoshi[1]; Hiroaki Takeda[1]; Mayu Hasegawa[2]; Junki Miyamoto[2]; Mikiko Takahashi[3]; Hiroshi Tsugawa[1, 3]; *[1]Tokyo University of Agriculture and Technology, Koganei-shi, Japan; [2]Tokyo University of Agriculture and Technology, Fuchu, Japan; [3]RIKEN Center for Sustainable Resource Science, Yokohama, Japan*

MP 484 **An Integrated MS-Based Platform for Structure-Based Identification and Quantification of Glycosphingolipids**; Ji Eun Park[1, 2]; Myung Jin Oh[1, 2]; Hyun Joo An[1, 2]; *[1]Chungnam National University, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea*

MP 485 **Identifying Oxidized Glycolipids in Microalgae: Bridging LC-MS Lipidomics with Biological Roles**; Rosario Domingues[1]; Tiago Conde[1]; Diana Lopes[1]; Tânia Melo[1]; Pedro Domingues[1]; *[1]University of Aveiro, Aveiro, Portugal*

MP 486 **Lipid Characterization Using MS Imaging and LCMS in Liver of a Metabolic Dysfunction-Associated Steatohepatitis (MASH) Mouse Model**; Doug Carlton[1]; Jeff Dahl[1]; Ruth Gordillo[2]; Toshiya Matsubara[1]; Christine Kusminski[2]; Kyounghee Min[2]; Philipp E Scherer[2]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]University of Texas Southwestern Medical Center, Dellas, TX*

MP 487 **Metabolic Degradation and Global Lipidome Incorporation of Polyfluorinated Model Decanes in Pseudomonas sp. Strain 273**; Alexander S Walls[1, 2]; Gao Chen[3, 4]; Diana Ramirez[3, 4]; Frank E Loeffler[3, 4, 5, 6]; Shawn R. Campagna[1, 2]; *[1]University of Tennessee Knoxville Chemistry Dept., Knoxville, TN; [2]Biological Small Molecule Mass Spectrometry Core, Knoxville, TN; [3]University of Tennessee, Knoxville, TN; [4]Department of Microbiology, Knoxville, TN; [5]Department of Civil and Environmental Engineering,* *Knoxville, TN; [6]Department of Biosystems Engineering and Soil Science, Knoxville, TN*

MP 488 **Efficient Multimodal MS Data Analysis with MZmine: Unraveling Lipid A Composition in Pathological E. coli**; Ansgar Korf[1]; Edward Rudt[2]; Steffen Heuckeroth[1]; Robin Schmid[3]; Tomáš Pluskal[3]; Heiko Hayen[2]; *[1]mzio GmbH, Bremen, Germany; [2]University of Münster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; [3]Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic*

MP 489 **Automated and detailed structural elucidation of lipids in biological matrix**; Pradeep Narayanaswamy[1]; Eva Duchoslav[2]; Pavel Ryumin[2]; *[1]SCIEX, Singapore, Singapore; [2]SCIEX, Concord, ON*

MP 490 **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[1]; Scott A. McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

MP 491 **Identification of positional isomers of linoleic acid containing phospholipids involved in pancreatic ductal adenocarcinoma**; Emily G Armitage[1]; Alan Barnes[1]; Elon Correa[2]; Sén Takeda[3]; Wen Chung[4]; Neil J Loftus[1]; *[1]Shimadzu Corporation, Manchester, United Kingdom; [2]Liverpool John Moores University, Liverpool, United Kingdom; [3]Department of Anatomy, Teikyo University School of Medicine, Tokyo, Japan; [4]Leicester HPB Unit, Glenfield Hospital, Leicester, United Kingdom*

MP 492 **Post Column Epoxidation for Differentiating Polar and Non-polar Lipids Isomers via Liquid Chromatography Co-axial Contained-ESI Mass Spectrometry**; Niraj K. Panday[1]; Alexander J. Grooms[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH*

MP 493 **A decision tree approach for triacylglycerol annotation of data-independent acquisition based lipidomics data**; Victor CL Lee[1]; Khanh CK Nguyen[1]; Thomas J Velenosi[1]; *[1]University of British Columbia, Vancouver, BC*

MP 494 **Large-scale lipidome analysis at the isomer-resolving level based on Omega Analyzer**; Junhan Wu[1]; Wenhui Pang[1]; Hongzheng Zhou[1]; Jiexun Bu[2]; Wenpeng Zhang[3]; Zheng Ouyang[3]; *[1]PURSPEC Technology(China) Ltd., Suzhou, China; [2]PURSPEC Technology (Beijing) Ltd., Beijing, China; [3]Tsinghua University, Beijing, China*

MP 495 **Evaluation of the synthesis of the branched chain ionizable lipid C12-200 using LC-MS/MS with low-energy electron impact fragmentation**; Daniel Zimmer[1]; Matthew D. Stone[2]; Robert Proos[2]; Santosh Kapil Kumar Gorti[2]; Christina Bailey-Hytholt[1]; *[1]Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MASSACHUSETTS; [2]SCIEX, USA, Framingham, MASSACHUSETTS*

MP 496 **Embrace both worlds: manipulating ion-types via gas-phase ion chemistry for structural elucidation of sugar-lipid conjugates**; Hsi-Chun Chao[1, 2]; Scott A. McLuckey[1]; *[1]Purdue University, West Lafayette, IN; [2]University of Illinois Urbana-Champaign, Champaign, IL*

MP 497 **Utilizing Normal Phase Amino Columns in Chromatography for Enhanced Discrimination of Charged, Chargedecayed, and Uncharged Modifications in Glycolipid and Glycan**; Akio Hayashi[1]; Takashi Matsuzaka[2]; Hitoshi Shimano[3]; *[1]Osaka University, Center for Infectious Disease Education and Research, Suita, Japan; [2]Department of Endocrinology and Metabolism, Faculty of Medicine, University of Tsukub, Tsukuba, Japan; [3]Department of Endocrinology and Metabolism, Faculty of Medicine, University of Tsukuba, Tsukuba, Japan*

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MP 498 **Tailored Cardiolipin Analysis in Complex Biological Matrices by two-dimensional HPLC coupled to high-resolution mass spectrometry**; Vera Schwantes[1]; Ann-Kathrin Weishaupt[2]; Julia Bornhorst[2]; Heiko Hayen[1]; *[1]University of Münster, Department of Inorganic and Analytical Chemistry, Münster, Germany; [2]University of Wuppertal, Faculty of Mathematics and Natural Sciences, Wuppertal, Germany*

MP 499 **Age-dependent changes in mouse brain and liver lipidomes**; Punyatoya Panda[1]; Christina R. Ferreira[2]; Allison Schaser[3]; Uma K. Aryal[1, 2]; *[1]Department of Comparative Pathobiology, Purdue University, West Lafayette, Indiana; [2]Bindley Bioscience Center, Purdue University, West Lafayette, Indiana; [3]Department of Speech, Language, and Hearing Sciences, Purdue University, West Lafayette, Indiana*

MP 500 **Bridging Gaps in Honey Bee Pheromone Analysis Using State-of-the-Art Lipidomics Analysis**; Armando Alcazar Magana[1, 2]; Alison McAfee[1, 3]; Shelley E. Hoover[4]; Leonard J Foster[1, 2]; *[1]Michael Smith Laboratories, Department of Biochemistry and Molecular Biology, University of British Columbia, Vancouver, British Columbia; [2]Life Sciences Institute, Department of Biochemistry and Molecular Biology, University of British Columbia, Vancouver, British Columbia; [3]Department of Applied Ecology, North Carolina State University, Raleigh, North Carolina; [4]Department of Biological Sciences, University of Lethbridge, Lethbridge, Alberta*

MP 501 **Untargeted Lipidomics of Murine Plasma Extracellular Vesicles**; Paul D Kennedy[1]; Brooke Saepoo[1]; Dilrukshika S.W. Palagama[2]; Miguel A. Gijon[1]; Elizabeth A. Hurst[1]; David LaGory[1]; *[1]Cayman Chemical Company, Ann Arbor, MI; [2]Cayman Chemical Company, Cayman Chemical Company, MI*

MP 502 **Investigating the Effects of Alteration in Lipid Profile on Biological Pathways in Diabetic Patients Treated with Different Drugs**; Waziha Tasnim Purba[1]; Shams Tarek Osman[2]; Oluwatosin Daramola[1]; Judith Nwaiwu[1]; Md Mostofa Al Amin Bhuiyan[1]; Mojibola Fowowe[1]; Junyao Wang[1]; Ahmed Elyazbi[3]; Yehia Mechref[1]; *[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; [2]Department of Clinical Pharmacy and Pharmacy Practice, Faculty of Pharmacy, Alexandria University, Alexandria, Egypt; [3]Department of Pharmacology and Therapeutics, Faculty of Pharmacy, Alamein International University, Alamein, Egypt*

MP 503 **High Throughput Profiling Method for Comprehensive Lipidomics Analysis of Samples of Limited Amounts**; Ya-Chun Chan[1]; Xiaohang Wang[1]; Shuang Zhao[1]; Liang Li[1]; *[1]The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta*

MP 504 **Effects of a High-Fat Diet on Triacylglycerols in Adipose Tissue in a GHSR KO Rat Model**; Lindsay A Kryszak[1]; Shelley N Jackson[1]; Andras H Leko[1]; Adriana Gregory-Flores[1]; Renata C N Marchette[1]; Janaina C M Vendruscolo[1]; Leandro F Vendruscolo[1]; Lorenzo Leggio[1]; *[1]National Institute on Drug Abuse, Baltimore, MD*

MP 505 **LC-MS Characterization of Lipid Nanoparticle Components and Relevant Major Cholesterol Oxidation Products**; Kevin Ray[1]; Katherine Sanders[1]; *[1]MilliporeSigma, St. Louis, MO*

MP 506 **Analyzing sex-dependent effects of bisphenol A on hepatic lipid metabolism in zebrafish using UPLC-Q-TOF/MS**; Won Noh; *Korea institute of Toxicology, Jinju, South Korea*

MP 507 **Time-dependent Investigation of Formation of Serum Biomolecular Coronas around Nanoparticles for Nanomedicine**; Gwi Ju Jang[1]; Min A Kim[1]; Heeju Joung[1]; Sang Yun Han[1]; *[1]Department of chemistry, Gachon University, Seongnam-si, South Korea*

MP 508 **Vendor-dependent mobile phase contaminants affect neutral lipid detection in lipidomics analyses**; Joshua A Roberts[1]; Angela S Radnoff[1]; Aleksandra Bushueva[1]; Jocelyn A Menard[1]; Karl V Wasslen[1]; Meaghan Harley[1]; Jeffrey M Manthorpe[1]; Jeffrey C Smith[1]; *[1]Department of Chemistry, Carleton University, Ottawa, ON*

MP 509 **MRM based free fatty acids profiling in human plasma using LC-MS/MS**; Yuki Suzuki[1]; Naoko Nagano[2]; Takahiro Goda[1]; Masaki Yamada[3]; *[1]SHIMADZU Corporation, Kawasaki, Japan; [2]Shimadzu General Services, Inc., Kyoto, Japan; [3]Shimadzu Corporation, Kyoto, Japan*

MP 510 **Distinct Polar Lipid Profiles in Fatty Acid Oxidation Disorders Identified by Dried Blood Spot Lipidomics**; Inês M. S. Guerra[1, 2]; Hugo Rocha[3, 4]; Tânia Melo[1, 2]; Ana S. P. Moreira[2]; M. Rosário Domingues[1, 2]; Pedro Domingues[1]; *[1]Mass Spectrometry Center, LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, Aveiro, Portugal; [2]CESAM- Centre for Environmental and Marine Studies-, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, , Portugal, Aveiro, Portugal; [3]Newborn Screening, Metabolism and Genetics Unit, Human Genetics Department, National Institute of Health Doutor Ricardo Jorge, Porto, Portugal; [4]Department of Pathological, Cytological and Thanatological Anatomy, School of Health, Polytechnic Institute of Porto, Porto, Portugal*

MP 511 **LIPIDOMICS OF SICKLE CELL DISEASE AND LIPID PROFILING OF ERYTHROCYTES-NOVEL FINDING**; Prasanth Kumar Punathil Kannan[1]; Sugasini Dhavamani[2]; Anuj Tiwari[3]; Jagadeesh Ramasamy[1]; *[1]Department of Pediatrics, University of Illinois at Chicago, Chicago, IL; [2]University of Illinois, Chicago, IL; [3]Discovery Partners Institute, Chicago, IL*

MP 512 **Non-targeted lipidomics of human plasma for discovering biomarkers in thrombogenesis**; Chau Tran[1]; Daniil G. Ivanov[1]; Sina Farzaneh[1]; Juan M. Jiménez[1]; Evgenii Serebriakov[1]; Igor A. Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

MP 513 **Differences in the diet of calves detected in beef samples using surface extraction and multiple reaction monitoring profiling of lipids**; Juliana A Torrecilhas[1]; Gislaine Dos Santos[2, 3]; Tiago J P Sobreira[3]; Sage Y Min[4]; Bruce R Cooper[3]; Rogerio A Curi[5]; Luis A Chardulo[1, 5]; Luciana M Sousa[1, 5]; Flavio D Resende[5]; Gustavo R Siqueira[5]; Guilherme L Pereira[1, 5]; Christina R Ferreira[3]; *[1]College of Veterinary and Animal Science, University of São Paulo State Júlio de Mesquita Filho, Botucatu, Brazil; [2]Department of Veterinary Medicine, College of Animal Sciences and Food Engineering, University of São Paulo, Pirassununga, Brazil; [3]Bindley Bioscience Center, Purdue University, West Lafayette, Indiana; [4]Department of Biomedical Engineering, Purdue University, West Lafayette, Indiana; [5]College of Agronomics and Veterinary Sciences, University of São Paulo State Júlio de Mesquita Filho, Jaboticabal, Brazil*

MP 514 **Untargeted Lipidomics Pipeline for 3rd Generation Lentiviral Vectors and Packaging Cells**; Jocelyn A Menard[1]; Joshua A Roberts[1]; Elena Godbout[2]; Christopher N Boddy[3]; Jean-Simon Diallo[2, 3]; Jeffrey C Smith[1, 4]; *[1]Department of Chemistry, Carleton University, Ottawa, ON; [2]Centre for Cancer Therapeutics, Ottawa Hospital Research Institute, Ottawa, ON; [3]Department of Chemistry and Biomolecular Sciences, Ottawa, ON; [4]Carleton Mass Spectrometry Centre, Carleton University, Ottawa, ON*

MP 515 **In vivo oxidized neural phospholipid detection and relative quantification using GC-MS/MS and LC-MS/MS**; Secilia Garza[1]; Genevieve James[1]; Hui Gyu Park[2]; Paul Baker[3]; Mikhail Shchepinov[4]; J. Thomas Brenna[1, 2]; *[1]University of Texas, Austin, TX; [2]Dell Pediatric Research Institute, University of Texas at Austin, Austin, TX; [3]SCIEX, Redwood City, CA; [4]BioJiva, LLC, Los Altos, California*

MP 516 **Phospholipid compositions of human lymphoma cells revealed by LC-MS/MS utilizing trapped ion mobility spectrometry**; Dominik M Wieland[1]; Heiko Hayen[1]; *[1]University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany*

MP 517 **A Multimodal Mass Spectrometry Approach to Profiling Sulfatides in Mouse Brains using the EAE Multiple Sclerosis Mouse Model**; Anastasiia Gordeeva[1]; Stephan B. Bach[1]; Krista Berlin[1]; Kayla Martinez[1]; *[1]University of Texas at San Antonio, San Antonio, TX*

MP 518 **Lipidomic profiling of the ER membrane upon activation of the unfolded protein response**; Bianca De Jonckheere[1, 2]; Paulina Kettel[3, 4]; Elif Karagöz[3, 5]; Robert Ahrends[1]; *[1]Institute of Analytical Chemistry, University of Vienna, Vienna, Austria; [2]University of Vienna, Vienna Doctoral School in Chemistry, Vienna, Austria; [3]Max Perutz Laboratories Vienna, Vienna BioCenter, Vienna, Austria; [4]Vienna BioCenter PhD Program, Doctoral School of the University of Vienna and Medical University of Vienna, Vienna, Austria; [5]Medical University of Vienna, Vienna, Austria*

MP 519 **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[1]; Janaina Isabel Mendoza Chaves[1]; Chad Weisbrod[2]; Marcela Nouzova[3]; Fernando Gabriel Noriega[3, 4, 5]; Francisco A Fernandez-Lima[1, 5]; *[1]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [2]National High Magnetic Field Laboratory, Florida State University, Thallahassee, FL; [3]Institute of Parasitology, Biology Centre CAS, Czech Republic; [4]Department of Biology Sciences, Florida International University, Miami, FL; [5]Biomolecular Sciences Institute, Florida International University, Miami, FL*

MP 520 **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; *Korea Institute of Toxicology, Jinju, South Korea*

MP 521 **Application of TIMS-MRMS to the study of lipids in human blood plasma**; Viola Jeck[1]; Alina Theisen[1]; Christopher Wootton[1]; Matthew R Lewis[2]; *[1]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359, Germany; [2]Bruker UK Limited, Life Sciences Mass Spectrometry Division, Coventry, United Kingdom*

MP 522 **Development of an Improved Folch Method for Simultaneous Extraction of Gangliosides and Lipids from microglia-derived extracellular vesicles**; Kimberly del Carmen Molina Bean[1]; Shawn N. Whitehead[2]; Adriana Zardini Buzatto[3]; Shuang Zhao[4]; Liang Li[4]; *[1]The Metabolomics Innovation Centre, Edmonton, AB; [2]Vulnerable Brain Laboratory, Dept. Anatomy and Cell Biology, Western University, London, Ontario; [3]University of Calgary, Calgary, AB; [4]University of Alberta, Edmonton, AB*

MP 523 **Paving the way toward analysis ofCaenorhabditis elegansindividuality – Development of single worm lipidomics based on nanoLC-TIMS-MS/MS** ; Narayanaganesh Balasubramanian[1]; Klidel Fae Rellin[2]; Lisa Abel[3]; Aiko Barsh[4]; Sven W Meyer[4]; Michael Witting[5]; *[1]Bruker Scientific, Fremont, CA; [2]Helmholtz Zentrum München German Research Center for Environmental Health, Neuherberg, Germany; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [5]Technical University of Munich, Freising, Germany*

MP 524 **Comprehensive data acquisition workflow on Orbitrap Astral MS for untargeted lipidomics to achieve deep lipidome coverage with high confidence annotations**; Rahul Ravi Deshpande[1]; Ciara Myer[1]; Bashar Amer[1]; Thomas Moehring[2]; Susan S Bird[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

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MP 525 **Interactions of the microbiome and radiation exposure: How may this affect emergency responses after a potential mass radiation exposure?**; Evan Pannkuk[1]; Igor Shuryak[2]; Anika Kot[1]; Lorreta Yun-Tien Lin[1]; Heng-Yong Li[1]; Albert J Fornace, Jr[1]; *[1]Georgetown University, Washington Dc, DC; [2]Columbia University Irving Medical Center, New York, NY*

MP 526 **Evaluation of clustering algorithms in small molecule tandem mass spectrometry**; Xianghu Wang[1]; Mingxun Wang[2]; *[1]University of California, Riverside, riverside, CA; [2]University of California, Riverside, Riverside, CA*

MP 527 **Identifying Metabolic Proliferation Mechanisms of IDH-dependent Cancer Using Liquid Chromatography-Mass Spectrometry Metabolomics**; Mathula Muhundan[1]; Olivia Taverniti[1, 2]; William D. Gwynne[1]; Andrew T. Quaile[1]; J. Rafael Montenegro-Burke[1, 2]; *[1]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; [2]Department of Molecular Genetics, University of Toronto, Toronto, ON*

MP 528 **Enabling Drug Development with Multi-Omics Integration of Host-Microbiome Crosstalk**; Cristina Di Poto[1]; Sukithar Rajan[2]; Xiang Tian[1]; Paul Warrener[3]; Oliver Fiehn[4]; Stewart MacArthur[5]; Erik L. Allman[1]; Sonja Hess[1]; *[1]Dynamic Omics, Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD; [2]Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Molndal, Gothenburg, Sweden; [3]Bacteriology, eV&I, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD; [4]West Coast Metabolomics Center, University of California Davis, Davis, CA; [5]Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Cambridge, United Kingdom*

MP 529 **Sequential target and Non-target for Global (STANG) metabolomics in discovering prognostic biomarkers of acute ischemic stroke**; Chao-Jung Chen[1]; Yu-Ning Lin[1]; *[1]China Medical University, Taichung, Taiwan*

MP 530 **Cell Metabolomics and Network Pharmacology: An Integrated Approach to Unravel the Potential Therapeutic Components of Astragalus radix for Allergic Rhinitis**; Akshay S Patil[1]; Yachun Shu[2]; Yan Xu[1]; *[1]Cleveland State university, CLEVELAND, OH; [2]Jiangsu Province Seaside Rehabilitation Hospital, Lianyungang, China*

MP 531 **Metabolomics Analysis of Adherent Mammalian Cells from 96-Well Culture Plates Using Automated Sample Preparation and LC-MS/MS MRM Profiling**; Edward S Folk[1]; Celeste Sandoval[1]; Sudha Gollapudi[1]; Christian John Ventura[1]; Ary Shalizi[1]; Phil Seitzer[1]; Alireza Delfarah[1]; Brian Feng[1]; Bryson Bennett[1]; *[1]Calico Life Sciences, South San Francisco, CA*

MP 532 **How does your HILIC method stack up? Optimization and comparison of common HILIC columns, mobile phases and additives for metabolomics**; Sierra D. Durham[1]; Karen E. Yannell[1]; Cate Simmermaker[1]; *[1]Agilent Technologies, Santa Clara, CA*

MP 533 **Assessing the metabolic impact of Toxoplasmosis correlating to immune response, parasite burden and the microbiome**; Caitlyn E Middleton[1]; Mahbobeh Lesani[2]; Tzu-Yu Feng[3]; Jan Carlos Urban Arroyo[3]; Eli Casarez[3]; Sarah Ewald[3]; Laura-Isobel McCall[1, 4]; *[1]Department of Chemistry and Biochemistry, San Diego State University, San Diego, CA; [2]Department of Microbiology and Plant Biology, University of Oklahoma, Norman, Oklahoma; [3]Department of Microbiology, Immunology and Cancer Biology at the Carter Immunology Center, University of Virginia School of Medicine, Charlottesville, Virginia; [4]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma*

MP 534 **Longitudinal study investigating serum metabolites and their association with type 2 diabetes risk in a Korean population**; Youngae Jung[1]; Geum-Sook Hwang[1]; *[1]Korea Basic Science Institute, Seoul, South Korea*

MP 535 **Metabolomic Profiling of Coffea canephora Coffees: An In-Depth Exploration of Maturation Influence by UHPLC-ESI(±)LTQ MS**; Marcos V. V. Lyrio[1, 2]; Henzo P. Salvador[3]; Danieli G. Debona[1]; Nayara A. dos Santos[2]; Fábio L. Partelli[3]; Wanderson Romão[2, 4]; Eustáquio V. R. De Castro[1]; *[1]Coffee Chemistry Laboratory - Coffee Design Group, Department of Chemistry, Federal University of Espírito Santo, Vitória, Brazil; [2]Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espirito Santo, Vitória, Brazil; [3]Department of Agrarian and Biological Sciences (DCAB), University Center of Northern Espírito Santo (CEUNES), Federal University of Espírito Santo, São Mateus, Brazil; [4]Federal Institute of Espírito Santo, Vitória, Brazil*

MP 536 **Increasing the detectability of phosphorylated metabolites by LC-HRMS/MS**; Kathrina Mae Kumaresan[1]; Nathan Ghafari[1]; Lekha Sleno[1]; *[1]University of Quebec in Montreal (UQAM), Montreal, QC*

MP 537 **Bridging High-Coverage Metabolomics Datasets and Overcoming Batch Effect Using a Universal Metabolome Standard**; Shuang Zhao[1]; Xiaohang Wang[1]; Rui Qin[1]; Liang Li[1, 2]; *[1]The Metabolomics Innovation Centre (TMIC), Edmonton, AB; [2]Department of Chemistry, University of Alberta, Edmonton, AB*

MP 538 **A system suitability scheme for assessment of longitudinal LC-TIMS-MS performance to promote reproducibility in omics sciences**; Erica Marie Forsberg[1]; Matthew R Lewis[2]; Ilmari Krebs[2]; Patrick Groos[2]; Jonas Wloka[2]; Stefan Harsdorf[2]; Sven W Meyer[2]; *[1]Bruker Daltonics, San Jose, CA; [2]Bruker Daltonics GmbH & Co. KG, Billerica, MA*

MP 539 **Single-Point External Calibration for Quantitative Metabolomics with a Novel Microchip CE-MS Platform Coupled to HRMS**; Katherine Raiche[1]; Sam Stewart[2]; Joshua P Guerrette[3]; Scott Mellors[3]; Erin Redman[3]; Corinne E Moss[4]; Katherine A Overmyer[5]; Joshua J Coon[4]; J. Will Thompson[3]; *[1]908 Devices, Boston, MA; [2]908 Devices Inc., Boston, MA; [3]908 Devices Inc., Morrisville, NC; [4]University of Wisconsin Madison, Madison, WI; [5]University of Wisconsin-Madison, Madison, WI*

MP 540 **Optimization of Analytical Methods for Metabolomics Studies of Samples Collected Using Microsampling Devices**; Tiffany T Trinh[1]; Ruiqi Jian[1]; Longsha Liu[1]; Lihua Jiang[1]; Linda Lan[1]; Michael P. Snyder[1]; *[1]Stanford University, Palo Alto, CA*

MP 541 **Routine Targeted Metabolomic Panel Analysis from Untargeted Acquisition of Differing Mouse Plasma Populations**; Cate Simmermaker[1]; Karen E Yannell[1]; Sierra D. Durham[1]; *[1]Agilent Technologies, Santa Clara, CA*

MP 542 **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 543 **LC-MS/MS Metabolomics of Induced Drosera capensis Digestion Reveals Broad Changes in the Abundance of Different Small Molecules**; Zane G Long[1]; Gemma R. Takahashi[2]; Jonathan V. Le[2]; Rachel W. Martin[1]; *[1]University of California, Irvine, Irvine, CA; [2]University of California Irvine, Irvine, CA*

MP 544 **Macrophage Infiltration in KRAS-Driven Lung Adenocarcinoma is driven by Lipid Metabolism and TAp73 Status**; Vanessa Y. Rubio[1]; Hayley D. Ackerman[1]; Nicole Hackel[1]; Jaden Baldwin[1]; John M. Koomen[1]; Elsa R. Flores[1]; *[1]Moffitt Cancer Center, Tampa, FL*

MP 545 **Effects of formic acid concentration and purity on chromatographic performance and ionization in untargeted metabolomics**; Nathan Montgomery[1]; Melanie T. Odenkirk[2, 3]; Chi-Ming Chien[2]; Jacqueline Michelle Chaparro[3, 4]; Margaret Read[3]; Sarah Brinkley[5, 6]; Katrina L Leaptrot[7]; Stacy D Sherrod[7]; Jody C May[7]; Cole Michel[8]; Katrina Doenges[8]; Arpana Vaniya[9]; John A McLean[7]; Richard Reisdorph[8]; Nichole Reisdorph[8]; Oliver Fiehn[9]; Tracy Shafizadeh[2]; Steve Watkins[2]; Jessica E Prenni[3]; Corey D Broeckling[4]; *[1]Colorado State University, Fort Collins, CO; [2]Verso Biosciences, Davis, CA; [3]Department of Horticulture and Landscape Architecture, Fort Collins, CO; [4]Analytical Resources Core: Bioanalysis and Omics Center, Colorado State University, Fort Collins, CO; [5]Department of*

Horticulture Sciences, Texas A&M University, College Station, TX; [6]CIAT Bioversity Alliance, Texas A&M University, College Station, TX; [7]Department of Chemistry and Center for Innovative Technologies, Vanderbilt University, Nashville, TN; [8]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of Colorado, Denver, CO; [9]West Coast Metabolomics Center, University of California Davis, Davis, CA

MP 546 **Comprehensive Metabolomic Analysis of Human Heart Tissue and Application to Diabetic Cardiomyopathy**; Benjamin Wancewicz[1]; Melissa R Pergande[1]; Yanlong Zhu[1]; Zhan Gao[1]; Zhuoxin Shi[1]; Kylie Plouff[1]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI*

MP 547 **Multi-site metabolomic reproducibility evaluation by LC-MS**; Rebecca Jones[1]; Caroline Chidley[2]; Xiaoyang Su[3]; Mirela Berisa[4]; Drew R Jones[1]; Ryan D Sheldon[5]; *[1]NYU Langone Health, New York, NY; [2]UMass Chan Medical School, Worchester, MA; [3]Rutgers University, New Brunswick, NJ; [4]Icahn School of Medicine at Mount Sinai, New York, NY; [5]Van Andel Institute, Grand Rapids, MI*

MP 548 **The development of a Human Metabolome Atlas uncovers metabolic signatures of hematological lineages**; Jeremy K Chan[1]; William D Gwynne[1]; Nicholas S Ly[1]; Brandon Y Lieng[1]; Olivia Taverniti[1]; Andrew T Quaile[1]; J. Rafael Montenegro-Burke[1]; *[1]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON*

MP 549 **MSTUS sample-to-sample Normalization has an interesting anomaly, yielding better normalizations**; Debasish Ghosh[1]; Vladimir Shulaev[1]; Chris Beecher[2]; Felice de Jong[3]; *[1]Department of Biological Sciences, College of Science, University of North Texas, Denton, Texas; [2]IROA Technologies LLC, Chapel Hill, North Carolina; [3]IROA Technologies LLC, Nellysford, VA*

MP 550 **Anion Exchange Chromatography Coupled with Orbitrap Mass Spectrometry for Simultaneous Quantitation and Discovery (SQUAD) Analysis of Organic Acids**; Justin Y Elliott[1]; Bashar Amer[2]; Susan S Bird[2]; Hussain Abdulla[1]; *[1]Texas A&M Corpus Christi, Corpus Christi, TX; [2]Thermo Fisher Scientific, San Jose, CA*

MP 551 **The influence of the microbiome on changes in the metabolome after T. cruzi infection**; Luis Ernst[1]; Laura-Isobel McCall[1]; Monica Ness[2]; Nathan Colwell[2]; Azadeh Nasuhidehnavi[2]; Morgan Harris[2]; Micah D`Armand De Chateauvieux[2]; *[1]San Diego State University, San Diego, CA; [2]University of Oklahoma, Norman, OK*

MP 552 **Development of a microflow metabolomics method for the detection of low-abundant metabolites**; Theodore Sana[1]; Rahul Deshpande[2]; Bashar Amer[3]; Susan S Bird[3]; Danya Dean[1]; Thomas Wyche[1]; *[1]Merck & Co., Inc., Cambridge, MA; [2]ThermoFisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Lexington, MA*

MP 553 **Application of Self Organizing Maps (SOM) to analyze the phenomenon of ion suppression**; Chris Beecher[1]; Felice A. De Jong[2]; Iqbal Mahmud[3]; Bo Wei[3]; Lucas Veillon[3]; Lin Tan[3]; Sara Martinez[3]; Bao Tran[3]; Alexander Raskind[1]; Rehan Akbani[3]; John N. Weinstein[3]; Philip L. Lorenzi[3]; *[1]IROA Technologies LLC, Chapel Hill, North Carolina; [2]IROA Technologies LLC, Nellysford, VA; [3]Department of Bioinformatics and Computational Biology at The University of Texas MD Anderson, Houston, Texas*

MP 554 **Evaluation of an easily adoptable microchip CE-MS metabolomics platform to quantify hundreds of metabolites from cells and tissues**; Aurora Cabrera[1]; Thomas S Webb[1]; Scott Lyons[1]; Jessica Thaxton[1]; Saame Raza Shaikh[1]; Erin A. Redman[2]; J. Will Thompson[2]; Laura Herring[1]; *[1]UNC-Chapel Hill, Chapel Hill, NC; [2]908 Devices Inc., Morrisville, NC*

MP 555 **Ion suppression correction and data normalization in metabolomics**; Iqbal Mahmud[1]; Bo Wei[1]; Lucas Veillon[1]; Lin Tan[1]; Sara Martinez[1]; Bao Tran[1]; Alexander Raskind[2]; Felice de Jong[2]; Rehan Akbani[1]; John N. Weinstein[1]; Chris Beecher[2]; Philip L. Lorenzi[1]; *[1]MD Anderson Cancer Center, Houston, TX; [2]IROA Technologies LLC, Chapel Hill, NC*

MP 556 **Mass spectra annotation using learned representations in the spectrum-molecule joint embedding space**; Apurva Kalia[1]; Soha Hassoun[1]; *[1]Tufts University, Medford, MA*

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MP 557 **High-Coverage Metabolomics Analyses Identifies Ameliorative Pathway and Metabolites for Manganese-induced Parkinson's Disease Phenotype and Neurotoxicity**; Yunjia Lai[1]; Pablo Reina-Gonzalez[2]; Gali Maor[3]; Gary W. Miller[1]; Souvarish Sarkar[2]; *[1]Columbia University, New York, NY; [2]University of Rochester, Rochester, NY; [3]Harvard Medical School, Boston, MA*

MP 558 **Tracing the Evolutionary Chemistry of Life through Mining of Public Metabolomics Data**; Yasin El Abiead[1]; Michael Strobel[2]; Lee R. Hagey[3]; Emily Gentry[4]; Helena Mannochio-Russo[3]; Paulo Wender P. Gomes[3]; Simone Zuffa[3]; Mingxun Wang[2]; Pieter C. Dorrestein[3, 5]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, UCSD, San Diego, CA; [2]UC Riverside, Riversdie, CA; [3]UC San Diego, La Jolla, CA; [4]Virginia Tech, Blacksburg, Virginia; [5]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

MP 559 **Metabolomics assisted breeding: a new approach for the development of new crop varieties**; Amancio J De Souza[1, 2]; Anil Bhatia[1, 2]; Haiyan Ke[1, 2]; Manhoi Hur[1, 2]; Andrew Huynh[1]; Philip A Roberts[1]; Bao Lam Huynh[1]; *[1]University of California Riverside, Riverside, CA; [2]UCR Metabolomics Core, University of California, Riverside, California*

MP 560 **GC-MS based metabolomics uncovered antioxidant pathways associated with curcumin supplementation in HepG2 induced oxidative stress**; Rossarin Tansawat[1, 2]; Nureesun Mahamad[3]; Ponsiree Jithavech[1]; Chawanphat Muangnoi[4]; *[1]Department of Food and Pharmaceutical Chemistry, Faculty of Pharmaceutical Sciences, Chulalongkorn University, Bangkok, Thailand; [2]Metabolomics for Life Sciences Research Unit, Chulalongkorn University, Bangkok, Thailand; [3]The Halal Science Center, Chulalongkorn University, Bangkok, Thailand; [4]Cell and Animal Model Unit, Institute of Nutrition, Mahidol University, Nakhon Pathom, Thailand*

MP 561 **Utilization of Monodisperse Fully Porous Particles for Chromatographic Improvement in Mass Spectrometry based Metabolomics for Disease Detection**; Geoff Faden[1]; Timothy J. Garrett[2]; Ed Faden[1]; *[1]MAC-MOD Analytical, Chadds Ford, PA; [2]University of Florida, Gainesville, FL*

MP 562 **A Dynamic Simultaneous Quantitation and Discovery (SQUAD) Liquid Chromatography Mass Spectrometry Approach for Inflammatory Bowel Disease Metabolomics in African Americans**; Jada S Gray[1]; Olatomiwa O Bifarin[1]; Samuel G. Moore[1]; David A. Gaul[1]; Sana Syed[2]; Adam Greene[2]; Jason Papin[2]; Gregory C Gibson[1]; Subra Kugathasan[3]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]University of Virginia, Charlottesville, VA; [3]Emory University School of Medicine, Atlanta, GA*

MP 563 **Evaluation of Tissues Preserved in RNAlater for Metabolomics Analysis**; Crystal L. Pace[1]; Bradley C. Cochran[1]; Richard J. Robinson[1]; *[1]Metabolon Inc., Morrisville, NC*

MP 564 **Investigating metabolic consequences of cigarette smoke exposure in murine lung tissue via untargeted metabolomics and cheminformatic approaches**; Kirsten E Overdahl[1]; Ezazul Haque[1]; Darryl C. Zeldin[1]; Stephanie J. London[1]; Alan K. Jarmusch[1]; *[1]National Institute of Environmental Health Sciences, Research Triangle Park, NC*

MP 565 **Performance evaluation of polarity switching for untargeted metabolomics using orbitrap mass spectrometer**; Hailemariam Abrha Assress[1, 2]; Mario G.

Ferruzzi[1, 2]; Colin D. Kay[1, 2]; Renny S. Lan[1, 2]; *[1]Arkansas Children's Nutrition Center, Little Rock, Arkansas; [2]Department of Pediatrics, University of Arkansas for Medical Sciences, Little Rock, Arkansas*

MP 566 **Untargeted metabolomics workflows using correlation analysis to uncover links between metabolic pathways**; Nathan Ghafari[1]; Lekha Sleno[1]; *[1]University of Quebec in Montreal, Montreal, QC*

MP 567 **Metabolomic analysis of single-spheroids based on chemical isotope labeling micro-flow liquid chromatography-mass spectrometry**; Cyrene Catenza[1]; Xian Luo[2]; Liang Li[1, 2]; *[1]University of Alberta, Edmonton, AB; [2]The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta*

MP 568 **Using a High Performance Four-Channel CIL LC-MS Method for Discovery of Metabolites Associated with Enteric Methane Emissions in Beef Cattle**; Xiaohang Wang[1]; Hongwei Li[2]; Michael Vinsky[3]; Ghader Manafiazar[2, 4]; Carolyn Fitzsimmons[2, 3]; Liang Li[5]; Changxi Li[2, 3]; *[1]The Metabolomics Innovation Centre (TMIC), Edmonton, AB; [2]Department of Agricultural, University of Alberta, Edmonton, AB; [3]Lacombe Research and Development Centre, Agriculture and Agri-Food Canada, Lacombe, AB; [4]Department of Animal Science and Aquaculture, Dalhousie University, Truro, NS; [5]Department of Chemistry, University of Alberta, Edmonton, AB*

MP 569 **Matrix Effect Evaluation using Post-Column Infused Standards for Hydrophilic Interaction Liquid Chromatography-Mass Spectrometry Method Development**; Mengle Zhu[1]; Pingping Zhu[1]; Pascal Maas[1]; Lieke Lamont[1]; Anne-Charlotte Dubbelman[1, 2]; Amy C. Harms[1]; Thomas Hankemeier[1]; *[1]Metabolomics and Analytics Centre, Leiden Academic Centre of Drug Research, Leiden University, Leiden, Netherlands; [2]Institute of Risk Assessment Sciences, Utrecht University, Utrecht, Netherlands*

MP 570 **Characterization of metabolome and lipidome cargo of extracellular vesicles**; Khyatiben Pathak[1]; Caitlyn Fain[1]; Melissa N. Martinez[1]; Patrick Pirrotte[1, 2]; *[1]Translational Genomics Research Institute, Phoenix, AZ; [2]City of Hope, Duarte, CA*

MP 571 **Bioactivity-Guided Functional Metabolomics: An Integrated LC-MS/MS Microfluidics-based Bioassay Approach**; Christian Geibel[1]; Simon Knoblauch[1]; Julian Schubert[1]; Albert Hernandez[1]; Keshab Bhattarai[1]; Giovanni Andrea Vitale[1]; Paolo Stincone[1]; Stilianos Papadopoulos Lambidis[1]; Jan Straetener[1]; Harald Gross[1]; Heike Brötz-Oesterhelt[1]; Daniel Petras[1, 2]; *[1]University of Tuebingen, Germany, Tuebingen, Germany; [2]University of California Riverside, Riverside, CA*

MP 572 **Absolute quantitation of metabolites in murine blood plasma using machine learning: a step towards generalizing to untrained analytes**; Luke S Ferro[1]; Alan Wong[2, 3]; Jack Howland[1]; Timothy Kassis[1]; Ana S.H. Costa[1]; Jefferson G. Pruyne[1]; Steven B Hooper[1]; Joshua D. Lauterbach[1]; Devesh Shah[1]; Mimoun Cadosch Delmar[1]; Jack Geremia[1]; Naama Kanarek[2, 3]; Jennifer M Campbell[1]; *[1]Matterworks, Somerville, MA; [2]Boston Children's Hospital, Boston, USA, MA; [3]Harvard Medical School, Boston, MA*

MP 573 **2-channels labeling and spatial distribution of metabolites in small amounts of fruits by micro-punches and LC-MS**; Vi Thanh Tran[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*

MP 574 **Using lipidomics to unravel metabolic pathways in Alzheimer's disease: a follow-up study**; Mariana S Marques[1, 2]; Leda Leme Talib[3]; Alessandra Sussulini[1, 2, 4]; *[1]State University of Campinas, Campinas, Brazil; [2]Laboratory of Bioanalytics and Integrated Omics (LaBIOmics), University of Campinas (UNICAMP), Campinas, Brazil; [3]Laboratory of Neurosciences LIM27, São Paulo, Brazil; [4]National Institute of Science and Technology of Bioanalytics (INCTBio), University of Campinas (UNICAMP), Campinas, Brazil*

MP 575 **Untargeted metabolomics for improved detection of bisphosphonate use in equine athletes**; Bethany C Keen[1, 2]; Fuyu Guan[1, 2]; Mary A Robinson[1, 2]; *[1]Department of Clinical Studies – New Bolton Center, School of Veterinary Medicine, University of Pennsylvania, Kennett Square, PA; [2]Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA*

MP 576 **Two Dimensional Liquid Chromatography Tandem Mass Spectrometry Reveals Microbial Metabolites in Host-Microbe Interactions**; Stilianos Papadopoulos Lambidis[1]; Claudia Mirretta Barone[1]; Dennis Jakob[1]; Daniel Petras[2, 3]; Ruth E Ley[1]; *[1]Department of Microbiome Science, Max Planck Institute for Biology, Tuebingen, Germany; [2]University of California, Riverside, RIVERSIDE, California; [3]Functional Metabolomics Lab, Cluster of excellence CMFI, University of Tuebingen, Tuebingen, Germany*

MP 577 **Non-targeted profiling of Nepeta Cataria using multidimensional gas chromatography, and high-performance mass spectrometry**; John Hayes[1]; David E Alonso[2]; Craig Fowler[1]; *[1]LECO Corporation, Saint Joseph, MI; [2]Leco Corporation, St. Joseph, MI*

MP 578 **Machine Learning Enhanced Direct Infusion Mass Spectrometry for High-throughput Metabolomics**; Arzu Tugce Guler[1]; Boryana Petrova[2]; Tamara Hadzic[3]; *[1]Institute for Experiential AI at Northeastern University, Boston, MA; [2]Boston Children's Hospital, Boston, MA; [3]Northeastern University, Boston, MA*

MP 579 **High-Throughput Screening of Bioengineered Microorganisms Using a "Fast-Pass" Desorption Electrospray Ionization-Mass Spectrometry Imaging Workflow**; Hawkins S Shepard[1]; Baltazar E Zuniga[1]; Joshua P Abraham[2]; Jody C May[1]; Brian F Pfleger[2]; Jamey D Young[1]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]University of Wisconsin-Madison, Madison, WI*

MP 580 **Exploring the Metabolome in Serum and Cerebrospinal Fluid of Traumatic Brain Injury Patients by LC-MS/MS**; Sarah A Sahioun[1]; Judith Nwaiwu[1]; Oluwatosin E Daramola[1]; Vishal Sandilya[1]; Cristian Gutierrez-Reyes[1]; Waziha Tasnim Purba[1]; Firas Kobeissy[2]; Stefania Mondello[3]; Ava M Puccio[4]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas; [2]Morehouse School of Medicine, Atlanta, Georgia; [3]University of Messina, Messina, Italy; [4]University of Pittsburgh, Pittsburgh, Pennsylvania*

MP 581 **Evaluation of automated detection of bile acid-amino acid conjugates in feces from a clinical study**; Stephen Barnes[1]; Landon Wilson[2]; Youngmee Kim[3]; *[1]University of Alabama at Birmingham, Birmingham, AL; [2]University of Alabama at Birmingham, Birmingham, Alabama; [3]University of Miami, Miami, FL*

MP 582 **COVID-19 unevenly impacts metabolism in the periphery of the coronal plane of the lungs**; Jarrod A Roach[1, 2]; Biyun Xue[3]; Jian Zheng[3]; Stanley Perlman[3]; Laura-Isobel McCall[2]; *[1]University of Oklahoma, Norman, OK; [2]San Diego State University, San Diego, CA; [3]University of Iowa, Iowa City, IA*

MP 583 **An Offline Two-dimensional LC-MS Platform for Rapid Metabolome Analyses of Complex Samples**; Sicheng Quan[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*

MP 584 **Achieving In-Depth Multi-omic Coverage of Exosomes through Systematic Comparison of Multiple Extractions and High-Resolution Mass Spectrometry**; Andrew J Perciaccante[1]; Melissa R Pergande[2]; Timothy J Aballo[2, 3]; Kevin M Buck[1]; Ying Ge[1, 2, 3]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [2]University of Wisconsin-Madison, Department of Cell and Regenerative Biology, Madison, WI; [3]University of Wisconsin-Madison, Molecular and Cellular Pharmacology Training Program, Madison, WI*

MP 585 **A metabolomics-guided approach for the identification of predictors of treatment response for rheumatoid arthritis**; Denise Marradi[1]; Camilla Dido'[1]; Elettra Barberis[2];

Pier Paolo Sainaghi[1]; Marcello Manfredi[1]; *[1]Department of Translational Medicine, University of Piemonte Orientale, Novara, Italy; [2]Department of Sciences and Technological Innovation, University of Piemonte Orientale, Alessandria, Italy*

MP 586 **Using molecular networking and explainable-AI to aggregate and interrogate untargeted metabolomics data for plant biology**; Manasa Appidi[1]; Sameer Mudbhari[1]; Dana L Carper[2]; Richard J Giannone[2]; Tomas Rush[2]; Doug Hyatt[2]; Daniel Jacobson[2]; Robert L Hettich[2]; Melissa Cregger[2]; John Field[3]; Udaya Kalluri[2]; Paul E Abraham[2]; *[1]UT-ORNL Graduate School of Genome Science and Technology, University of Tennessee, Knoxville, TN, USA, Knoxville, TN; [2]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; [3]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN*

MP 587 **Developing and Implementing a Signal Handling Approach for More Accurate Metabolite Elemental Composition Determination using Orbitraps**; Chia-Wei Hsu[1]; Wei-Hung Chang[1]; Ya-Wen Chou[1]; Yet-Ran Chen[1]; *[1]Academia Sinica, Taipei, Taiwan*

MP 588 **Assess Poly and Perfluoroalkyl Substances (PFASs) using untargeted metabolomics in the Child Health and Development Studies**; Dongxue Wang[1]; Nickilou Y. Krigbaum[2]; Piera M. Cirillo[2]; ViLinh Tran[3]; Dean P. Jones[3]; Barbara A. Cohn[2]; Xin Hu[1]; *[1]Rollins School of Public Health, Emory University, Atlanta, GA; [2]The Center for Research on Women and Children's Health, Public Health Institute, Berkeley, California; [3]School of Medicine, Emory University, Atlanta, GA*

MP 589 **A Comprehensive Study on the Regulation of Compound Zaoren Granule on Metabolic Disorder in CUMS-PCPA induced Insomnia Rats**; Yachun Shu[1, 2]; Zekun Wang[1]; Yajun Chen[3]; *[1]Affiliated Hospital of Nanjing University of Chinese Medicine, Nanjing, China; [2]Jiangsu Province Seaside Rehabilitation Hospital, Lianyungang, China; [3]Nanjing Women and Children's Healthcare Hospital, Nanjing, China*

MP 590 **Empowering Research: Constructing a Comprehensive Untargeted Metabolomics Pipeline for Dynamic Microbiome Research**; Jessica C Little[1, 2]; Michael Mullowney[1, 2]; Eric Pamer[1, 2]; Ashley Sidebottom[1, 2]; *[1]Duchossois Family Institute, Chicago, IL; [2]University of Chicago, Chicago, IL*

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MP 591 **Proteomic profiling to study the effect of light on Pseudomonas aeruginosa biofilms**; Lipi Das[1, 2]; Kelly N. Eckartt[1]; Alexander W. Rookyard[1, 2]; Lars E. P. Dietrich[1]; Lewis M. Brown[1, 2]; *[1]Department of Biological Sciences, Columbia University, New York, NY; [2]Quantitative Proteomics and Metabolomics Center, Columbia University, New York, NY*

MP 592 **Legacy effects of plant–soil feedbacks under drought on drought tolerance of post-succeeding soybean plants**; Yushiro Fuji[1]; Megumi Narukawa[2]; Mai Tsuda[3]; Yasunori Ichihashi[2]; Ryosuke Sasaki[1]; Yui Nose[2]; Kengo Sakurai[4]; Hirokazu Takahashi[5]; Hideki Takanashi[4]; Yoshihiro Omori[4]; Akito Kaga[6]; Hisashi Tsujimoto[7]; Mikio Nakazono[5]; Toru Fujiwara[4]; Hiroyoshi Iwata[4]; Masami Hirai[1]; *[1]RIKEN Center for Sustainable Resource Science, Yokohama, Japan; [2]RIKEN BioResource Research Center, Tsukuba, Japan; [3]Tukuba Univ. Tsukuba-Plant Innovation Research Center, Tsukuba, Japan; [4]Grad. Sch. Agr. Life Sci., Univ. Tokyo, Bunkyo-ku, Japan; [5]Grad. Sch. Bioagric. Sci., Nagoya Univ., Nagoya, Japan; [6]Inst. Crop Sci., NARO, Tsukuba, Japan; [7]Arid Land Res. Ctr., Tottori Univ., Tottori, Japan*

MP 593 **Lipid characterization along the zebrafish body-axis and isolated intestine using High-Resolution MALDI Imaging mass spectrometry**; Jacquelyn Spathies[1]; Caitlin Murdoch[2, 3]; Madeline E Colley[4, 5]; Lukasz Migas[5, 6]; Eric Skaar[2, 3]; Raf Van De Plas[4, 5, 6]; Jeffrey M Spraggins[3, 4, 5, 7, 8]; *[1]Vanderbilt University, Nashville, TN; [2]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; [3]Vanderbilt Institute for Infection, Immunology and Inflammation, Vanderbilt University School of Medicine, Nashville, Tennessee; [4]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [5]Department of Biochemistry, Vanderbilt University, Nashville, TN; [6]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [7]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN; [8]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN*

MP 594 **Ferric Ion-based Surface-assisted Laser Desorption/Ionization Mass Spectrometry for the Analysis of Small Molecules and Microorganisms**; Tzu Ling Yang[1]; Chih-Wei Chen[1]; Yu-Chie Chen[1]; *[1]National Yang Ming Chiao Tung University, Hsinchu, Taiwan*

MP 595 **A binary-matrix applied in the study of bacteria**; Xinhua Guo; *Jilin University, Changchun, China*

MP 596 **Deciphering the microbiome: a targeted LC/MS/MS method for the comprehensive analysis of bile acids in biological samples**; Pietro Morlacchi[1]; Ruben J.F. Ramos[2]; Christophe Deckers[3]; Limian Zhao[3]; Mark Sartain[3]; Daniel Cuthbertson[3]; Justin R Cross[2]; *[1]Agilent Technologies, Inc., Lexington, MA; [2]Memorial Sloan Kettering Cancer Center, New York, NY; [3]Agilent Technologies, Inc., Santa Clara, CA*

MP 597 **The Peptonizer2000 for taxonomic identification of metaproteomic samples with a new taxonomic quantification method**; Tanja Holstein[1, 2]; Pieter Verschaffelt[2, 3]; Lennart Martens[2, 4]; Thilo Muth[5]; *[1]Ghent University, Gent, Belgium; [2]VIB-UGent Center for Medical Biotechnology, Gent, Belgium; [3]Ghent University, Ghent, Belgium; [4]Gent University, Gent, Belgium; [5]Robert Koch Institute, Berlin, Germany*

MP 598 **Non-invasive diagnosis of mixed invasive pulmonary aspergillosis and mucormycosis**; Dominika Luptáková[1]; Rutuja H. Patil[2]; Radim Dobiáš[3]; Milan Navrátil[4]; David A. Stevens[5]; Vladimír Havlíček[1]; *[1]Institute of Microbiology, Prague 4, Czech Republic; [2]Institute of Microbiology of the Czech Academy of Sciences, 142 20, Prague, Czech Republic; [3]Public Health Institute, Ostrava, Czech Republic; [4]Department of Haematooncology, University Hospital Ostrava and Faculty of Medicine, University of Ostrava, Ostrava, Czech Republic; [5]Stanford University, Stanford, CA*

MP 599 **Proteomic characterization of a Haematococcus pluvialis (Chlorophyceae) mutant with a higher heterotrophic growth rate**; Kyarii Ramarui[1]; Jun Zhong[2]; Yantao Li[1]; *[1]University of Maryland Center for Environmental Science, Institute of Marine and Environmental Technology, Baltimore, MD; [2]Mayo Clinic, Rochester, MN*

MP 600 **Non-targeted Metabolomics enables the Identification of Keystone Specialised Metabolites in a Phyllosphere derived Synthetic Microbial Community Model**; Paolo Stincone[1, 2]; Vasvi Chaudhry[2]; Karoline Steuer-Lodd[3]; Lukas Miles Braun[2]; Monja Schmid[2]; Franziska Höhn[1]; Nadine Ziemert[1]; Eric Kemen[2]; Daniel Petras[1, 3]; *[1]University of Tuebingen, Interfaculty Institute of Microbiology and Infection Medicine, Tuebingen, Germany; [2]University of Tuebingen, Center for Plant Molecular Biology, Tübingen, Germany; [3]University of California, Riverside, Riverside, CA*

MP 601 **Tackling the identification challenge in metaproteomics**; Tim Van Den Bossche[1]; Justine Lemaître[1]; Lennart Martens[1]; *[1]VIB-UGent Center for Medical Biotechnology, VIB, Ghent, Belgium*

MP 602 **Integrative mass spectrometry based workflow to study drug resistance against aminoglycosides in Escherichia coli**; Nilanjan Ghosh Dastidar[1]; Nicola S. Freyer[1]; Ingo Wohlgemuth[1]; Henning Urlaub[2, 3]; Marina V. Rodnina[1]; *[1]Department of Physical Biochemistry, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; [2]Bioanalytical Mass Spectrometry Group, Max Planck*

Institute for Multidisciplinary Sciences, Göttingen, Germany; [3]Institute of Clinical Chemistry, Bioanalytics, University Medical Center Göttingen, Göttingen, Germany

MP 603 **Investigating the impact of different chemicals on the gut microbiota in vitro**; Vittoria F Borrini[1]; Denise Marradi[2]; Riccardo Nuzzi[2]; Virginia Vita Vanella[2]; Marco Ghirimoldi[2]; Beatrice Purghè[2]; Francesco Dondero[1]; Elettra Barberis[1]; Marcello Manfredi[2]; *[1]Department of Sciences and Technological Innovation, University of Piemonte Orientale, Alessandria, Italy; [2]Department of Translational Medicine, University of Piemonte Orientale, Novara, Italy*

MP 604 **Gut microbial metabolic pathways as opportunities for new therapeutic strategies in cardiometabolic diseases**; Ina Nemet[1]; Xinmin S. Li[1]; Arash Haghikia[2, 3, 4]; Lin Li[1]; Jennifer Wilcox[1]; Kymberleigh A Romano[1]; Jennifer A Buffa[1]; Marco Witkowski[1]; Ilja Demuth[2, 5]; Maximilian König[2]; Elisabeth Steinhagen-Thiessen[2]; Fredrik Bäckhed[6]; Michael Fischbach[7, 8]; W.H. Wilson Tang[1, 9]; Ulf Landmesser[2, 3, 4]; Stanley L Hazen[1, 9]; *[1]Department of Cardiovascular & Metabolic Sciences and Center for Microbiome & Human Health, LRI, Cleveland Clinic, Cleveland, OH; [2]Charité-Universitätsmedizin, Berlin, Germany; [3]German Center for Cardiovascular Research, (DZHK), Germany; [4]Berlin Institute of Health, (BIH), Germany; [5]Berlin Institute of Health Center for Regenerative Therapies, Berlin, Germany; [6]University of Gothenburg, Gothenburg, Sweden; [7]ChEM-H Institute and Departments of Bioengineering and Microbiology and Immunology, Stanford University, Stanford, CA; [8]Chan Zuckerberg Biohub, San Francisco, CA; [9]Heart, Vascular, and Thoracic Institute, Cleveland Clinic, Cleveland, OH*

MP 605 **Characterization of extracellular vesicules of intestinal microbiota using metaproteomics in patients with Crohn's disease**; Celine HENRY[1]; Maxime Long[1]; Valentin Loux[2]; Romain Sausset[1]; Catherine Juste[1]; Marianne De Paepe[1]; *[1]Université Paris-Saclay, INRAE, AgroParisTech, Micalis Institute, Jouy-en-Josas, France; [2]Université Paris-Saclay, INRAE, MaIAGE, Jouy-en-Josas, France*

MP 606 **A metaproteome assessment of microbiome changes following microbial invasion**; Dana L Carper[1]; Alyssa A Carrell[1]; Leah H Burdick[1]; Dale A Pelletier[1]; Paul E Abraham[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN*

MP 607 **Community Curation of Microbiome Metabolites for The Mechanistic Analysis of Metabolomics Data**; Helena Mannochio-Russo[1]; Shipei Xing[1]; Fernanda De Oliveira[1, 2]; Wilhan D Gonçalves Nunes[3]; Martijn Van Faassen[4]; Vincent Charron-Lamoureux[1]; Sydney Thomas[1]; Paulo Wender Portal Gomes[1]; Marilyn De Graeve[5]; Haoqi Nina Zhao[1]; Irina Koester[6]; Ralph Riley Torres[6]; Nicole E Avalon[6]; Simone Zuffa[1]; Andrés Mauricio Caraballo-Rodríguez[1]; Yasin El Abiead[1]; Ipsita Mohanty[1]; Lucia Cancelada[6, 7]; Felipe Vasquez-Castro[1]; Sarolt Magyari[8]; Mingxun Wang[9]; Pieter C Dorrestein[1, 10, 11, 12]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [2]Engineering School of Lorena, University of Sao Paulo, Lorena, Brazil; [3]Federal Institute of Education, Science and Technology of São Paulo, Ilha Solteira, Brazil; [4]University Medical Center Groningen, University of Groningen, Groningen, Netherlands; [5]Department of Translational Physiology, Infectiology and Public Health, Ghent University,, Merelbeke, Belgium; [6]Scripps Institution of Oceanography, University of California, San Diego, CA; [7]Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA; [8]Institute of Microbiology, ETH, Zurich, Switzerland; [9]Department of Computer Science, University of California Riverside, Riverside, CA; [10]Center for Microbiome Innovation, University of California San Diego, La Jolla, CA; [11]Department of Pharmacology, University of California San Diego, La Jolla, CA; [12]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

MP 608 **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[1]; Feng Xian[1]; Christoph Krips[2]; Manuela Schmidt[1]; *[1]University of Vienna, Vienna, Austria; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

MP 609 **Meta-omic analysis of anaerobic microbiomes digesting senescent switchgrass across a gradient of pH, temperature, and retention times**; Michael Shreve[1]; Dana L Carper[2]; Katharine Strandquist[1]; Payal Chirania[3]; Ikenna O Okekeogbu[2]; Robert L Hettich[2]; John M Regan[1]; Tom L Richard[1]; Richard J. Giannone[2]; *[1]The Pennsylvania State University, University Park, PA; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]The University of Tennessee Knoxville, Knoxville, TN*

MP 610 **The Solution is in Sourdough: Harnessing Microbial Diversity for Unique Chemical Composition of Bread**; Eva G Keohane[1]; Jacqueline M Chaparro[1]; Melanie Odenkirk[1]; Arpana Vaniya[2]; Josephine Wee[3]; Charlene Van Buiten[1]; Jessica E Prenni[1]; *[1]Colorado State University, Fort Collins, CO; [2]West Coast Metabolomics Center, University of California Davis, Davis, CA; [3]Pennsylvania State University, State College, Pennsylvania*

MP 611 **MALDI and DART mass spectrometry analysis of a single entity microorganism attached to a disk electrode**; Luciana V Rivera Molina[1]; Gabriela Campos[1]; Tyler C Arntz[1]; Aliaksei Boika[1]; Chrys Wesdemiotis[1]; *[1]University of Akron, Akron, OH*

MP 612 **Targeted UHPLC-LC-MS/MS elucidates microbially derived metabolism following xanthohumol supplementation in adults with active Crohn's Disease**; Paige Jamieson[1]; Jan F Stevens[2]; Thomas O. Metz[3]; Ryan Bradley[4]; *[1]Oregon State University, Corvallis, OR; [2]Oregon State University, Corvallis, Oregon; [3]Pacific Northwest National Laboratory, Richland, WA; [4]National University of Natural Medicine, Portland, Oregon*

MP 613 **Temporal cysteine redox proteome profiling of engineered Synechococcus elongatus PCC 7942 cscB/SPS in the context of circadian disruption**; Xiaolu Li[1]; Pavlo Bohutskyi[1]; Natalie C Sadler[1]; Austin Gluth[2]; Marina A Gritsenko[1]; Song Feng[1]; Tong Zhang[1]; Margaret S Cheung[3]; Wei-Jun Qian[1]; *[1]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [2]Washington State University, Pullman, WA; [3]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA*

MP 614 **Metabolomic profiling of aromatic amino acid-derived lactic acids in fermented foods**; Megan Danielewicz[1]; Ryan Lieb[1]; Allis Chien[1]; Sean Spencer[2]; Justin L Sonnenburg[2]; *[1]Stanford University Mass Spectrometry, Stanford, California; [2]Stanford University, Stanford, CA*

MP 615 **Impact of Sample Complexity on Measurement Dynamic Range in Microbiome Proteomics**; Megan K Elliott[1, 2]; Samantha L Peters[2]; Robert L Hettich[2]; Richard J Giannone[2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN*

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MP 616 **Assessment of HILIC-MS in characterizing mixtures of duplexed siRNAs**; Ming Huang[1]; Haibo Qiu[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals Inc., Tarrytown, NY*

MP 617 **mRNA Oligonucleotide Characterization via Low Flow Ion Pair-Reversed Phase Chromatography and Tandem Mass Spectrometry (LF-IP-RP-MS/MS)**; Roxana Eggleston-Rangel[1]; Jason Anspach[1]; Michael McGinley[1]; *[1]Phenomenex, Torrance, CA*

MP 618 **From discovery to quantitative profiling of RNA modifications using template-directed RNA cleavage and bioinformatics analysis of MS2 spectra**; Anna Popova[1]; Xiyu Dong[1]; Farshad Abdollah-Nia[1]; Nikhil Jain[2];

Robert A. Britton[2]; James R. Williamson[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Baylor College of Medicine, Houston, Texas*

MP 619 **From ASOs to tRNA: Comprehensive Sequence Characterization of Highly Modified Oligonucleotides by low Mathieu q resonant CID Based Dissociation Methods**; Joshua D Hinkle[1]; Robert L Ross[2]; William M McGee[2]; Scott Kronewitter[2]; Ping Yip[2]; John E.P. Syka[1]; James L Stephenson Jr[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Lexington, Massachusetts*

MP 620 **Characterization of G-Quadruplexes using CID, 213 nm UVPD, and a-EPD**; Jessica G Pauling[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

MP 621 **Quantitative Proteomics Identifies Profilin-1 As A Pseudouridine-binding Protein**; Songbo Wei[1]; Jun Yuan[2]; Shiyuan Guo[2]; Zheng Duan[1]; Jernej Murn[2]; Yinsheng Wang[2]; *[1]University of California Riverside, Riverside, CA; [2]University of California, Riverside, Riverside, CA*

MP 622 **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[1]; Leif Morin[1]; Aihua Liu[1]; *[1]Resolian (Formally Alliance Pharma), Malvern, PA*

MP 623 **Optimizing Sample Preparation, Chromatography, and Informatics for Improved Sequence Coverage of mRNA Therapeutics by LC/MS/MS**; Michael d Mcginley[1]; Roxana Eggleston-Rangel[1]; Alyssa Nodland[1]; *[1]Phenomenex, Torrance, CA*

MP 624 **A quantitative proteomics approach for the identification of reader proteins of pseudouridine in RNA**; Andrew H Kellum Jr[1]; Xiaochen Liang[1]; Xiaochuan Liu[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

MP 625 **Development of a Microflow IPRP UHPLC-MS/MS method for improved quantitative analysis of therapeutic oligonucleotides in human plasma**; Hao Yang[1]; Min Du[2]; Neloni R. Wijeratne[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Lexington, MA*

MP 626 **Distinguishing Steroisomers of the Cyclobutane Pyrimidine Dimer Photoproduct by Ion Mobility Mass Spectrometry and MS/MS**; Hsin-Chieh Yang[1]; Savannah Scruggs[1]; Mengqi Chai[1]; John-Stephen Taylor[1]; Michael L. Gross[1]; *[1]Washington University in Saint Louis, St. Louis, MO*

MP 627 **Synthesis and characterizations of oligodeoxynucleotides containing site-specifically incorporated carboxymethyl phosphotriester and assessment of their formation in DNA**; Garrit M Clabaugh[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

MP 628 **Development of a flow-through-based limited RNase T1 digestion approach for high-throughput and high sequence-coverage mapping of therapeutic mRNAs**; Shuli Tang[1]; Gaoyuan Liu[1]; Yuetian Yan[1]; Shunhai Wang[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY*

MP 629 **High Resolution Mass Spectrometry and LC-UV Data Streams Applied to Characterizing Oligonucleotide Impurities**; Kosuke Uchiyama[1]; Noriko Kato[1]; Takeshi Nomura[1]; Hiroyuki Yasuda[1]; Simon Ashton[2]; Richard Price[2]; Helen Jose[2]; Neil Loftus[2]; Kiyoshi Kakiya[3]; Kazutoshi Kishi[3]; Yuka Fujito[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Corporation, Manchester, United Kingdom; [3]Peptistar Inc., Settsu, Japan*

MP 630 **Simultaneous Quantitation of 13 RNA Nucleotides Using Hydrophilic Interaction Chromatography Coupled With Triple Quadrupole Mass Spectrometry**; Roger E Moore[1]; Khyatiben Pathak[2]; Patrick Pirrotte[1, 2]; *[1]City of Hope, Duarte, CA; [2]Translational Genomics Research Institute, Phoenix, AZ*

MP 631 **Investigating the deamination of cytosine oxidation products in duplex DNA using isotopic labeling and LC-MS/MS**; Gabriel Robert[1]; Valentin Adelmard[1]; Guru Madugundu[1]; J Richard Wagner[1]; *[1]Université de Sherbrooke, Sherbrooke, QC*

MP 632 **Evaluation of Rationally Designed Compounds Targeting DNA Trinucleotide Repeat Expansions by Native Mass Spectrometry**; Raihana Afroz[1]; Jillian Berko[2]; Nana A. Acheampong[2]; Michael K. Berko[2]; Aliza N. Aslam[2]; Sarah B. Krueger[2]; Varun V. Gadkari[1]; *[1]University of Minnesota, Twin Cities, Minneapolis, MN; [2]Mount St. Mary's University, Frederick, MD*

MP 633 **Application of internal Standard MSMS quantification with oligonucleotide pharmaceuticals**; Christopher Gawlig[1]; Güngör Hanci[1]; Michael Ruehl[1]; *[1]BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany*

MP 634 **Comprehensive investigation of parameters influencing oligonucleotide mass spectra following IP-RP-separation and negative polarity ionization**; Till Wehner[1]; Christopher Gawlig[1]; Michael Ruehl[1]; *[1]BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany*

MP 635 **Capillary flow ion pair reversed-phase separation for very sensitive oligonucleotide LC-HRMS analysis and characterisation**; Ulrik H. Mistarz[1]; Shanhua Lin[2]; Shane L. Bechler[2]; Brandon H. Robson[2]; Ken Cook[3]; *[1]Thermo Fisher Scientific, Allerød, Denmark; [2]Thermo Fisher Scientific, Sunnyvale, CA; [3]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*

MP 636 **Sensitive detection of post transcriptional modifications in tRNA by microflow UHPLC-HRAM-MS/MS**; Shweta Chhajed[1]; Robert L Ross[1]; *[1]Thermo Fisher Scientific, Lexington, MA*

MP 637 **Metabolite Profiling of the Antisense Oligonucleotide Tofersen Using UHPLC-HRAM mass spectrometry**; Robert L Ross[1]; Keeley Murphy[1]; Stephane Houel[1]; Min Du[1]; *[1]Thermo Fisher Scientific, Lexington, MA*

MP 638 **mRNA critical quality attribute analysis using a UPLC-TOF MS System and customized software**; Ying-Qing Yu[1]; Rebecca J. D'Esposito[1]; Catalin E Doneanu[1]; Leslie Napoletano[1]; *[1]Waters Corporation, Milford, MA*

MP 639 **The Use of Chromatography, Ion Mobility, and Statistical Analyses to Characterize the Diastereomeric Composition of Phosphorothioated Oligonucleotides**; Mohsin Ali[1]; Sondos H. Abdelhafeez[2]; Ahmed M. Abdel-Megied Ali[3]; Michael P. Cummings[2]; Jace W. Jones[1]; *[1]School of Pharmacy, University of Maryland, Baltimore, MD; [2]University of Maryland, Department of Biology, College park, MD; [3]School of Pharmacy, Department of Pharmaceutical Sciences, Norte Dame University of Maryland, Baltimore, MD*

MP 640 **Simplifying eukaryotic transfer RNA Modification Mapping via FPLC**; Aastha Gyawali[1]; Patrick A Limbach[2]; *[1]University of Cincinnati, cincinnati, OH; [2]University of Cincinnati, Cincinnati, OH*

MP 641 **Characterization of RNA Chemical Modifications by HILIC coupled with Tandem Mass Spectrometry**; Qishan Lin[1]; Thomas Begley[1]; *[1]University at Albany, Albany, NY*

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MP 642 **Rapid Sequencing of Peptide Mixtures using Two-Dimensional Tandem Mass Spectrometry and Graph Partitioning Algorithms**; My Phuong Le[1]; Yu Zhu[1]; David F. Gleich[1]; Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN*

MP 643 **Fragmentation pattern of double derivatized protonated peptides (H3 model peptide) by high-resolution mass spectrometry**; Leila Afjehi[1, 2]; Benjamin Garcia[3]; *[1]University of Vienna, Vienna, Austria; [2]Research Support Facility, Mass spectrometry unit, Vienna, Austria; [3]Washington University School of Medicine, St. Louis, MO*

MP 644 **Cleavable biotin-alkyne outperforms uncleavable biotin-alkyne in the identification and quantification of newly**

synthesized proteins; Daniel B. Mcclatchy[1]; John R. Yates III[1]; *[1]Scripps Research, La Jolla, CA*

MP 645 **Comparison of dissociation techniques for the structural characterization of GLP-1 agonists using HRMS/MS**; Rachel Dicken[1]; Kirk Gaston[1]; *[1]US FDA, Cincinnati*

MP 646 **Combining Microdroplet reactions with ExD fragmentation for fast characterization of proteins and antibody subunits**; Thomas E Walker[1]; Rachel Franklin[2]; Joseph Meeuswen[2]; Jim Lau[3]; *[1]Agilent Technologies, Lexington, MA; [2]Agilent Technologies, Corvallis, Oregon; [3]Agilent Technologies, Wilmington, DE*

MP 647 **Current Role of Mass Spectrometry in Detecting Sequence Variants to facilitate Cell Line Development of Biotherapeutics**; Andrew D Mahan[1]; Haichuan Liu[2]; Zoe Zhang[2]; Hirsh Nanda[3]; *[1]Johnson and Johnson, Spring House, PA; [2]SCIEX, Redwood City, CA; [3]Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania*

PEPTIDES: PTM IDENTIFICATION
648-674

MP 648 **TIMAHAC: Streamlined Tandem IMAC-HILIC Workflow for Simultaneous and High-Throughput Analysis of Plant Phosphoproteomics and N-glycoproteomics**; Chin-Wen Chen[1]; Pei-Yi Lin[1]; Ying-Mi Lai[2]; Miao-Hsia Lin[3]; Shu-Yu Lin[4]; Chuan-Chih Hsu[1]; *[1]Institute of Plant and Microbial Biology, Academia Sinica, Taipei city, Taiwan; [2]Agricultural Biotechnology Research Center, Academia Sinica, Taipei city, Taiwan; [3]Department of Microbiology, National Taiwan University College of Medicine, Taipei city, Taiwan; [4]Academia Sinica Common Mass Spectrometry Facilities for Proteomics and Protein Modification Analysis, Academia Sinica, Taipei city, Taiwan*

MP 649 **Complimentary TIMS and ECD for Online Bottom-Up Histone Proteoform Elucidation**; Cassandra N Fuller[1]; Kevin Jeanne Dit Fouque[1]; Lilian Valadares Tose[1]; Francisca N De Luna Vitorino[2]; Benjamin A Garcia[2]; Francisco A Fernandez-Lima[1]; *[1]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [2]Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, St. Louis, MO*

MP 650 **Developing a MS-based Proteomics Approach to Study the Forms of ADP-ribosylation**; Isabel R Uribe[1]; Emily Zahn[2]; Benjamin A Garcia[2]; Ben Orsburn[1]; Anthony KL Leung[1]; *[1]Johns Hopkins University, Baltimore, MD; [2]Washington University in St. Louis, St. Louis, MO*

MP 651 **Histone Tyrosine Sulfation: Artifact or Reality?**; Menatallah M. Youssef[1, 2]; Miriam F. Ayad[2]; Lobna A. Hussein[2]; Maha F. Abdel-Ghany[2]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Faculty of Pharmacy, Ain Shams University, Cairo, Egypt*

MP 652 **Temporal Phosphoproteomics Analysis of HIV-1 Reactivation from Latency**; Yennifer Delgado[1, 2, 3]; Sara Makanani[1, 2, 3]; Vivian Yang[1, 2]; Erin Kim[1, 2]; Prashant Kaushal[1, 2, 3]; Oliver Fregoso[1, 2]; Mehdi Bouhaddou[1, 2, 3]; *[1]University of California, Los Angeles, Los Angeles, CA; [2]Department of Microbiology, Immunology, and Molecular Genetics, Los Angeles, CA; [3]Institute for Quantitative and Computational Biosciences, UCLA, Los Angeles, CA*

MP 653 **Global detection and quantification of viral protein post-translational modifications**; Prashant Kaushal[1, 2]; Mehdi Bouhaddou[1, 2]; *[1]Department of Microbiology, Immunology, and Molecular Genetics, Los Angeles, CA; [2]Institute for Quantitative and Computational Biosciences, UCLA, Los Angeles, CA*

MP 654 **Fast disulfide mapping by integrating programmable online disulfide-ene reaction onto the bottom-up protein analysis workflow**; Keting Zhou[1]; Yu Xia[1]; *[1]Tsinghua University, Beijing, China*

MP 655 **High-throughput simultaneous quantification of glycopeptides and phosphopeptides enabled by 12-plex DiLeu isobaric tags and dual-functional Ti(IV)-IMAC**; Feixuan Wu[1]; Danqing Wang[2, 3]; Dylan Nicholas T Tabang[2, 4]; Haiyan Lu[1]; Peng-Kai Liu[5]; Zicong Wang[1]; Yuan Liu[1, 6]; Lingjun Li[1, 2]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Genentech, South San Francisco, CA; [4]Boston Children's Hospital, Boston, USA, MA; [5]Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI; [6]Columbia University, New York, New York*

MP 656 **Differentiation of peptide epimers and its application to D-amino acid position determination using higher-energy collisional dissociation mass spectrometry**; Yuan-Chih Chen[1]; Hsin-Yi Wu[2]; Lung-Cheng Lin[3]; Chih-Wei Chang[1]; Pao-Chi Liao[1]; *[1]National Cheng Kung University, Tainan, Taiwan; [2]National Taiwan University, Taipei City, Taiwan; [3]ScinoPharm Taiwan, Ltd., Tainan, Taiwan*

MP 657 **Exploring the O-Sulfation Patterns in Endogenous CCK Peptides by Trapped Ion Mobility Spectrometry**; Elena V Romanova[1]; Alisha Doda[2]; James Checco[2]; Jonathan Sweedler[1]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL; [2]University of Nebraska - Lincoln, Lincoln, NE*

MP 658 **Differentiation of near-isobaric cysteine-modified peptides using LC-(IM)/MS/MS**; Sarah J Jones[1, 2]; Christopher J. Clarke[1, 2]; Philip J. Brownridge[1, 2]; Andrew R. Jones[1, 3]; Christoph Krisp[4]; Claire E. Eyers[1, 2]; *[1]University of Liverpool, Liverpool, United Kingdom; [2]Centre for Proteome Research, Liverpool, United Kingdom; [3]Computational Biology Facility, Liverpool, United Kingdom; [4]Bruker Daltonics, Bremen, Germany*

MP 659 **Source-induced dissociation (SID) coupled to FAIMS improves higher-energy collisional dissociation (HCD)-dependent fragmentation of ADP-ribose peptides**; Taku Kasai[1]; Masanori Aikawa[1, 2, 3]; Sasha A. Singh[1]; *[1]Center for Interdisciplinary Cardiovascular Sciences, Division of Cardiovascular Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA; [2]Center for Excellence in Vascular Biology, Cardiovascular Division, Brigham and Women's Hospital, Harvard Medical School, Boston, MA; [3]Channing Division of Network Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA*

MP 660 **New strategy for identification of various lipid modified PTMs from complex peptide solutions using SDC acid precipitation**; Martin R. Larsen[1]; Peter Toft Jensen[1]; Arkadiusz Nawrocki[1]; *[1]Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense M, Denmark*

MP 661 **Improving the Depth and Reliability of Glycopeptide Identification Using Protein Prospector**; Peter R. Baker[1]; Reuben Hogan[1]; Robert Chalkley[1]; *[1]UCSF, San Francisco, CA*

MP 662 **Systematic Robustness Testing, Linearity, Repeatability and Specificity of a Multi-attribute Method (MAM) for Biopharmaceutical Characterization and Prequalification**; Kiran Iyer; *Just Evotec Biologics, Seattle, WA*

MP 663 **N-SPyCE-enabled Delineation of Cell State-Dependent Changes to the N-terminome**; Alexandra C Turmon[1]; Andrew P Becker[1]; Alexander W Sun[1]; Lisa Boatner[1]; Nithesh Perumal[1]; Keriann M Backus[1]; *[1]University of California Los Angeles, Los Angeles, CA*

MP 664 **Improved peptide search for identification of SUMO2/3 and ubiquitin**; Caroline Lennartsson[1]; Ivo A Hendriks[1]; Jurgen Cox[2]; Michael L Nielsen[1]; *[1]Novo Nordisk Center for Protein Research, Copenhagen N, Denmark; [2]Max Planck Institute of Biochemistry, Martinsried, Germany*

MP 665 **TUPAX: Method development for the investigation of non-canonical phosphorylation**; Leonard A Daly[1, 2]; Christopher J. Clarke[1, 2]; Dominic P Byrne[2]; Philip J. Brownridge[1, 2]; Andrew J Alpert[3]; Patrick A Eyers[2]; Claire E Eyers[1, 2]; *[1]Centre for Proteome Research, Liverpool, United Kingdom; [2]University of Liverpool, Liverpool, United Kingdom; [3]PolyLC Inc, Columbia, MD*

MP 666 **Peptide mapping of tryptic digests for mAbs using a novel ExD cell on the 6545XT LC/Q-TOF mass spectrometer**; Stephen Sciuto[1]; Maozi Liu[1]; Rachel Franklin[2]; Jerry Han[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Corvallis, Oregon*

MP 667 **High throughput DIA analysis of histone PTMs using ZenoTOF**; Jaison Arivalagan[1]; Jessica Moore[1]; Danielle Gutierrez[1]; *[1]Discovery Life Sciences, Huntsville, AL*

MP 668 **A New Framework for Systematic Evaluation of Post-translational Modification Site Localization Approaches**; Pisit Wajanasara[1, 2, 3]; Nuno Bandeira[1, 2, 3, 4]; *[1]University of California San Diego, La Jolla, CA; [2]Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; [3]Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; [4]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

MP 669 **Development and optimization of mass spectrometry-based methods for site-specific identification of ADP-ribosylation**; Sara C Buch-Larsen[1]; Ivo A Hendriks[1]; Martin Rykær[1]; Michael L Nielsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen N, Denmark*

MP 670 **Comparative Analysis of Glycoproteomic Software Tools Using a Tailored Glycan Database**; Reuben Hogan[1]; Robert Chalkley[2]; Nicholas M. Riley[3]; Lauren E Pepi[4]; Nevan Krogan[2]; *[1]University of California, San Francisco, San Francisco, CA; [2]UCSF, San Francisco, CA; [3]University of Washington, Seattle, WA; [4]Beth Israel Deaconess Medical Center, Boston, MA*

MP 671 **Targeting Post-Translational Modifications on Herpesvirus Proteins to Eradicate Latent Infection**; Sara K. Makanani[1, 2]; Prashant Kaushal[1, 2]; Pu-Lin Teng[3]; Ting-Ting Wu[3]; Mehdi Bouhaddou[1, 2]; *[1]Department of Microbiology, Immunology, and Molecular Genetics, UCLA, Los Angeles, CA; [2]Institute for Quantitative and Computational Biosciences, UCLA, Los Angeles, CA; [3]Department of Molecular and Medical Pharmacology, UCLA, Los Angeles, California*

MP 672 **Untargeted characterization of substitution errors in hyper-accurate and error-prone bacterial ribosome mutant strains**; Taylor J. Lundgren[1]; Patricia L. Clark[1]; Matthew M. Champion[1]; *[1]University of Notre Dame, Notre Dame, IN*

MP 673 **Intensity-based site localization of post-translational modifications utilizing predicted peptide fragmentation spectra**; Michael Graber[1]; Alexander Hogrebe[1]; Daniel P Zolg[1]; Markus Schneider[1]; Tobias Schmidt[1]; Vishal Sukumar[1]; Florian Seefried[1]; Siegfried Gessulat[1]; Martin Frejno[1]; *[1]MSAID, Garching, Germany*

MP 674 **Improved Liquid Chromatography and MS/MS Methods for Sulfopeptide Identification**; Luke M Collier[1]; Menatallah M. Youssef[1, 2]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Faculty of Pharmacy, Ain Shams University, Cairo, Egypt*

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MP 675 **Mass Spectrometry evaluation of glycosylation variants and SP2/0 Host Cell Proteins during downstream processes: the case of an immunocytokine**; Ettore Gilardoni[1]; Lorenzo Ghezzi[2]; Emiliano Sani[2]; Riccardo Stucchi[1]; Dario Neri[2, 3]; *[1]Philochem AG, Otelfingen, Switzerland; [2]Philogen S.p.A., Sovicille, Italy; [3]Swiss Federal Institute of Technology, Department of Chemistry and Applied Biosciences, Zurich, Switzerland*

MP 676 **Targeted Absolute Quantification of Residual Host Cell Proteins using LC-MS/MS and Stable Isotope Labeled Peptide Standards**; Qiyao Li[1]; Anthony Blaszczyk[1]; Derrick Zhang[1]; Niomi R Peckham[1]; Zarema Kassymbek[1]; Jack Simpson[1]; *[1]United States Pharmacopeial Convention, Rockville, MD*

MP 677 **A High Throughput LC-MS Method for Cell Culture Media Nutrient and Metabolite Analysis Supporting Upstream Bioprocessing**; Yun Alelyunas[1]; Josh Gray[2]; Courtney Walton[1]; Guillaume Bechade[3]; Mark Wrona[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Immerse Labs, Newark, DE; [3]Waters Corporation, Wilmslow, United Kingdom*

MP 678 **Evaluating Traditional Mass Spectrometry Against the New Generation of Emerging Analytical Technology**; Nicole A Azer[1]; Xin Bush[1]; Nicholas Trunfio[1]; Erica Berilla[1]; Casey Kohnhorst[1]; David Naoki Powers[1]; *[1]US Food and Drug Administration, Silver Spring, MD*

MP 679 **Qualitative and quantitative proteomics of “high-risk” host cell proteins in monoclonal antibody bioprocessing using a novel 3M membrane technology**; Romel Dator[1]; Katie Stock[1]; Aaron Marcella[1]; Christine Hitomi[2]; Caitlin Wold[2]; David Chau[2]; Jennifer Heitkamp[2]; *[1]Materials, Life Sciences & Analytical, 3M Health Care Business Group, 3M Center, St. Paul, MN; [2]Separation and Purification Sciences Division, 3M Health Care Business Group, 3M Center, St. Paul, MN*

MP 680 **Applying UHPLC-HRAM MS/MS/MS method to assess host cell protein clearance during the purification process development of therapeutic mAbs**; Reiko Kiyonami[1]; Ying Chen[2]; Al De Leon[2]; Min Du[1]; *[1]Thermo Fisher Scientific, Lexington, MA; [2]Thermo Fisher Scientific, Bedford, MA*

MP 681 **Characterization of spent growth media and intracellular metabolites of CHO cells using a turnkey microchip CE-HRMS based workflow**; Erin Redman[1]; Awab Nehala[2]; Stephanie R. Klaubert[2]; Milla Neffling[2]; J. Will Thompson[1]; *[1]908 Devices Inc., Morrisville, NC; [2]908 Devices Inc., Boston, MA*

MP 682 **Optimization of a Mass Spectrometry Data Acquisition Method for Enhanced Detection of Amino Acid Misincorporations**; Nhu Q Vu[1]; Jun Zhang[1]; *[1]Amgen, Thousand Oaks, CA*

MP 683 **Streamlined top-down, middle-down, and bottom-up MS characterization of biotherapeutics on a single LC-MS platform**; Ivy Kia Ngee Low[1]; Yee Jiun Kok[1]; Xuezhi Bi[1, 2, 3]; *[1]Bioprocessing Technology Institute, Agency for Science, Technology and Research, Singapore, Singapore; [2]Duke-NUS Medical School, Singapore, Singapore; [3]Singapore Institute of Technology, Singapore, Singapore*

MP 684 **Understanding the Correlation between MAM and Conventional Product Quality Assays Through Multivariate Data Analysis**; Tingting Jiang[1]; Francis Kwofie[1]; Nick Attanasio[1]; Matthew Haas[1]; John Higgins[1]; Hari Kosanam[1]; *[1]Merck & Co., Inc., West Point, PA*

MP 685 **Development of a streamlined cell culture metabolite profiling assay using a new nominal mass hybrid mass spectrometer**; Elsa Gorre[1]; Bo Zhai[1]; Andrew D Mahan[1]; Sven Hackbusch[2]; Cristina Jacob[2]; Min Du[3]; *[1]Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Lexington, MA*

MP 686 **Accelerating biologic process development: Rapid Media Screening through AI/ML-Powered LC-MS Metabolomic Analysis with Universal Calibrators**; Jared Kress[1]; Tingting Jiang[1]; John Higgins[1]; Jack Howland[2]; Ana S.H. Costa[2]; Luke S Ferro[2]; Joshua D. Lauterbach[2]; Jefferson G. Pruyne[2]; Devesh Shah[2]; Timothy Kassis[2]; Jennifer M Campbell[2]; Hari Kosanam[1]; *[1]Merck & Co., Inc., West Point, PA; [2]Matterworks, Inc., Somerville, MA*

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687-722

MP 687 **A Novel, Proteome-based Cell Type Set Enrichment Analysis (pCtSEA)**; Casimir Bamberger[1]; Salvador Martinez De Bartolome[2]; Sandra Pankow[1]; Jolene K. Diedrich[1]; Robin Park[1]; John R. Yates III[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Yatiri Biosciences, San Diego, CA*

MP 688 **Quantifying Coupled Equilibria Using Slow Mixing Mode (SLOMO) Native Mass Spectrometry**; Duong T. Bui[1]; Elena N. Kitova[1]; Lara K. Mahal[1]; John S. Klassen[1]; *[1]University of Alberta, Edmonton, AB*

MP 689 **Determining the quaternary dynamics of small heat-shock proteins using Orbitrap charge detection-mass spectrometry**; Olav A. Johannessen[1]; Dominik Saman[1]; Justin L. P. Benesch[1]; *[1]Department of Chemistry, University of Oxford, Oxford, United Kingdom*

MP 690 **Mass spectrometry identification of LVV-H7 binding partners in response to alcohol dependence**; Marek Smoluch[1]; Kinga Hartman[1]; Anna Drabik[1]; Joanna Helena Kotlinska[2]; Silberring Jerzy[1]; Przemyslaw Mielczarek[1, 3]; *[1]AGH University of Krakow, Kraków, Poland; [2]Department of Pharmacology and Pharmacodynamics, Medical University of Lublin, Lublin, Poland; [3]Laboratory of Proteomics and Mass Spectrometry, Maj Institute of Pharmacology, Polish Academy of Sciences, Kraków, Poland*

MP 691 **Exploring Interactions Between Differently Charged LL-37 Variants and Lipids by Native Mass Spectrometry**; Til Erik Kundlacz[1]; Carla Schmidt[2]; *[1]Martin Luther University Halle-Wittenberg, Halle (Saale), Germany; [2]Johannes Gutenberg University, Mainz, Germany*

MP 692 **Native Mass Spectrometry Provides Insight into the Stability and Subunit Exchange Mechanism of Mutant Transthyretin Tetramers**; Carter Lantz[1]; Robert Rider[1]; Sangho Yun[1]; David Russell[1]; *[1]Texas A&M University, College Station, TX*

MP 693 **Using affinity purification mass spectrometry to interrogate TEAD protein interactions in cancer**; Alissa Guarnaccia[1]; Philamer Calses[1]; Victoria Pham[1]; Meena Choi[1]; Anwesha Dey[1]; Jennie Lill[1]; *[1]Genentech, South San Francisco, CA*

MP 694 **Advances in UniDec Software for Biotherapeutic Characterization**; Michael Thomas Marty[1]; Wilson Phung[2]; Wendy Sandoval[2]; *[1]University of Arizona, Tucson, AZ; [2]Genentech Inc, South San Francisco, CA*

MP 695 **Enzyme Catalysis in the Gas Phase Revealed by ESI-IMS/MS**; Yuen Ki Ng[1]; Elnaz Aliyari[1]; Caroline Cui[1]; Lars Konermann[1]; *[1]The University of Western Ontario, London, ON*

MP 696 **Synaptobrevin-2 shows a preference for negatively charged lipids**; Julia Bieber[1]; Carla Schmidt[1]; *[1]Johannes Gutenberg University, Mainz, Germany*

MP 697 **Use of native mass spectrometry to characterize the binding of substrate and inhibitors to Salmonella FraB deglycase, a drug target**; Yuan Gao[1, 2]; Jamison Law[1, 3]; Venkat Gopalan[1, 3]; Vicki H. Wysocki[1, 2, 3]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Native Mass Spectrometry Guided Structural Biology Center, Ohio State University, Columbus, OH; [3]Center for RNA Biology, Ohio State University., Columbus, OH*

MP 698 **LiP-MS guided drug discovery using the cancer driver Ras as a model system**; Foroughsadat Absar[1]; Evgeniy V. Petrotchenko[1]; Roopa Thapar[2]; Edith Nagy[2]; Jason B. Cross[2]; Christoph H. Borchers[1, 3, 4, 5]; *[1]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [2]M.D. Anderson Cancer Center, Institute for Applied Cancer Science, Therapeutics Discovery Division, Houston, TX; [3]Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; [4]Division of Experimental Medicine, McGill University, Montreal, QC; [5]Department of Pathology, McGill University, Montreal, QC*

MP 699 **Investigating the DNA binding behaviors and inhibition for human Rad52-DNA binding domain by native mass spectrometry and surface-induced dissociation**; Zihao Qi[1, 2]; Charles E. Bell[1, 3]; Vicki H. Wysocki[1, 2]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH; [3]Department of Biological Chemistry and Pharmacology, The Ohio State University, Columbus, OH*

MP 700 **Integrating Metabolic Glycan Phenotype Manipulation with Affinity Purification for a Systematic Exploration of Glycoprotein Interaction Networks**; Xingyu Liu[1]; Yixuan (Axe) Xie[1]; Siyu Chen[2]; Zongtao Lin[1]; Sheng Ying[2]; Shunyang Wang[2]; Carlito B. Lebrilla[2]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO; [2]UC Davis, Davis, CA*

MP 701 **Unraveling the Specificity of Membrane Protein-Lipid Interactions Using Mutant Cycling and Native MS**; Hiruni S Jayasekera[1]; Madison De Jesus[1]; Katherine Mae Miller[1]; Michael Thomas Marty[1]; *[1]The University of Arizona, Tucson, AZ*

MP 702 **Elucidating novel regulatory lncRNA-protein interactions in hematopoiesis by hybridization capture and mass spectrometry**; Yuling Dai[1]; Isabella Whitworth[1]; Brian Frey[1]; Mabel Minji JUNG[1]; Jeong-Ah Kim[1]; Emery H. Bresnick[1]; Lloyd M Smith[1]; *[1]University of Wisconsin-Madison, Madison, WI*

MP 703 **Allosteric Activation of AMP-Activated Protein Kinase Quantified using Native Mass Spectrometry**; Liam Bandura[1]; Boris Krichel[2, 3]; Matther S Fisher[1]; Emily A Chapman[1]; Ying Ge[1, 2, 4]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin; [2]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [3]School of Life Sciences, University of Siegen, Siegen, Germany; [4]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*

MP 704 **Systematic analysis of protein interactions using PrISMa**; Gunnar Dittmar[1]; Daniel Perez-Hernandez[1]; Sophie Rodius[1]; Marta Lavouras Mendes[1]; Mattson Jones[1]; *[1]Luxembourg Institute of Health, Strassen, Luxembourg*

MP 705 **Residue-specific mapping of the PD-1 epitope of nivolumab using X-ray footprinting mass spectrometry**; Line G. Kristensen[1]; Yan Chen[1]; Christopher J. Petzold[1]; Sayan Gupta[1]; Corie Y. Ralston[1]; *[1]Lawrence Berkeley National Laboratory, Berkeley, CA*

MP 706 **Understanding the recruitment mechanisms of peripheral membrane proteins through direct nativeMS analysis from tunable organellar-mimicking membranes**; Rachel A McAllister[1]; Wonhyeuk Jung[1]; Moitrayee Bhattacharyya[2]; Kallol Gupta[1]; *[1]Yale School of Medicine, Department of Cell Biology, New Haven, CT; [2]Yale School of Medicine, Department of Pharmacology, New Haven, CT*

MP 707 **Meltome-assisted profiling of protein complexes: Prediction of protein-protein interactions by cellular thermal shift assay and its application on malaria parasites**; Samuel Pazicky[1]; Seth Tjia[1]; Ka Diam Go[1]; Nicolas Aranciaga[1]; Zbynek Bozdech[1]; *[1]School of Biological Sciences, Nanyang Technological University, Singapore, Singapore*

MP 708 **Tracking Transient Protein-Protein Interactions in Targeted Protein Degradation using Proximity-Dependent Labeling Coupled to Mass Spectrometry**; Shu You[1]; Kristina Ivanov[1]; Duc Tran[1]; Clark Peterson[1]; Craig Stumpf[1]; Alex Campos[1]; *[1]Plexium, San Diego, CA*

MP 709 **Protein Fishing for the identification of interacting proteins: Identification of novel binding partners of Bri2 BRICHOS**; Helene Tigro[1]; Alexey Lyashkov[2]; Mohammed Khadeer[2]; Ruth Shimmo[1]; Luigi Ferrucci[2]; Janne Johansson[3]; Ruin Moaddel[2]; *[1]Tallinn University, Tallinn, Estonia; [2]NIA/NIH, Baltimore, MD; [3]Karolinska Institutet, Solna, Sweden*

MP 710 **Developing a computational pipeline to study dynamic cell processes under a changing proteome**; Julia Kitaygorodsky[1, 2]; Reuben Samson[1, 2]; Martina Tersigni[1]; Payman Samavarchi-Tehrani[1]; Christopher Go[1, 2]; Queenie Hu[1]; William R. Hardy[1]; Anne-Claude Gingras[1, 2]; *[1]Lunenfeld-Tanenbaum Research Institute Mount Sinai Hospital,* *Toronto, Ontario; [2]Department of Molecular Genetics, University of Toronto, Toronto, ON*

MP 711 **Optimizing proximity proteomics on the EvoSep-timsTOF LC-MS system**; Brendon Seale[1]; Julia Kitaygorodsky[1, 2]; Reuben Samson[1, 2]; Martina Tersigni[1]; Zhen-Yuan Lin[1]; Cassandra Wong[1]; Vesal Kasmaeifar[1, 2]; Anne-Claude Gingras[1, 2]; *[1]Lunenfeld-Tanenbaum Research Institute, Toronto, ON; [2]University of Toronto, Toronto, ON*

MP 712 **Analysis of protein complex stability and missense protein sequence variants associated with neurodegenerative disease**; Avery M Runnebohm[1]; HR Sagara Wijeratne[1]; Whitney Smith-Kinnaman[1]; Emma H Doud[1]; Amber L Mosley[1]; *[1]Indiana University School of Medicine, Indianapolis, IN*

MP 713 **Structural, Binding Site, and Functional Comparison of PCSK9 Inhibitors Discovered Utilizing a Natural Product Drug Discovery MS Platform**; Samantha J Knott[1]; Erik DeBloois[1]; Pelle Simpson[1]; William Old[1]; Marvin Yu[1]; Kurt Morgenstern[1]; Erik Zimmerman[1]; *[1]Enveda Biosciences, Boulder, CO*

MP 714 **Structure and Interactions of the Endogenous Human Commander Complex**; Markku Varjosalo; *HiLIFE, University of Helsinki, Helsinki, Finland*

MP 715 **Lactoferrin Interaction with Glycosaminoglycans studied with Native Mass Spectrometry**; Ruolan Cheng[1]; Daniil G. Ivanov[1]; Yi Du[1]; Igor A. Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

MP 716 **Heterogeneous Non-Canonical Inflammasome Oligomerization Probed by Narrow Quadrupole Selections and Electron Capture Charge Reduction**; Philip Lacey[1]; Chengliang Wang[2]; Jianbin Ruan[2]; Vicki H Wysocki[1]; *[1]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio; [2]The University of Connecticut Health, Farmington, Connecticut*

MP 717 **Monitoring Fe-S cluster synthesis on E. coli protein complex IscS-IscU using time-resolved native mass spectrometry**; Emily Burningham[1]; Shelby Oney-Hawthorne[1]; Cheng-Wei Lin[2]; David Barondeau[1]; David Russell[1]; *[1]Texas A&M University, College Station, TX; [2]Genentech Inc., South San Francisco, CA*

MP 718 **Experimental and Computational Methods for Increasing Coverage of Global Protein-Protein Interaction Networks in Dynamic Contexts**; Tavis J Reed[1]; Peter J Metzger[1]; Matthew D Tyl[1]; Alicja Tadych[1]; Olga G Troyanskaya[1]; Ileana M Cristea[1]; *[1]Princeton University, Princeton, NJ*

MP 719 **The Big Break Up—Understanding Why a Subunit or Polypeptide Abandons its Noncovalent Complex**; Rachel O. Loo[1]; Jessie Le[1]; Boyu Zhao[1]; Joseph A. Loo[1]; *[1]Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA*

MP 720 **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[1]; Sarah C Beno[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

MP 721 **Developing a Complex-centric XL-MS approach to Delineate the Human Interactome**; Sean Tang[1]; Clinton Yu[1]; Fenglong Jiao[1]; Lan Huang[1]; *[1]University of California-Irvine, IRVINE, CA*

MP 722 **A novel E3technology enables efficient, effective, and economical analysis of proteomes and protein-RNA interactions**; Yanbao Yu[1]; Ahmed Abdelgawad[1]; Guotao Lu[2]; Gregory A Davision[2]; Mona Batish[1]; *[1]University of Delaware, Newark, DE; [2]CDS Analytical LLC, Oxford, PA*

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MP 723 **Optimizing Digestion Efficiency: Impact of Various Denaturing Reagents on a 60-Biomarker Health Surveillance Panel in Human Plasma**; Erika Hernandez[1]; Dragana Noe[1]; Nathan Hendricks[1]; Susan M. Mockus[1]; *[1]Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA*

MP 724 **A Rapid, Reproducible, and Automated cIEF-ESI-MS Method for High-Throughput Top-Down Proteomic Analysis of Nanoparticle Protein Corona**; Reyhane Tabatabaeian Nimavard[1]; Guijie Zhu[2]; Amirhossein Sadeghi[2]; Liangliang Sun[2]; *[1]-Michigan State University, -East Lansing, MI; [2]Michigan State University Department of Chemistry, East Lansing, MI*

MP 725 **Higher dynamic range MS1 acquisition methods with parallel narrow isolation window DIA or DDA on an Orbitrap Astral mass spectrometer**; Ulises Hernandez Guzman[1]; Christian Thoeing[2]; Max Hoek[2]; Nicolaie Eugen Damoc[2]; Jesper Velgaard Olsen[1]; *[1]NovoNordisk Center for Protein Research, København, Denmark; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 726 **Accelerating Deep Proteome Sequencing with Orbitrap Astral**; John S Chlystek[1]; Annie Jen[1]; Pavel Sinitcyn[2]; Katherine A Overmyer[1, 2, 3]; Scott T Quarmby[1, 3]; Joshua J Coon[1, 2, 3, 4]; *[1]University of Wisconsin-Madison, Department of Biomolecular Chemistry, Madison, WI; [2]Morgridge Institute for Research, Madison, WI; [3]National Center for Quantitative Biology of Complex Systems, Madison, WI; [4]University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin*

MP 727 **Connecting the Dots: A Closer Look at Cleavage Preferences of Proline Semi-Specific Endopeptidases**; Zuzana Kalaninova[1, 2]; Jasmina M Portasikova[1, 2]; Barbora Jireckova[1, 2]; Daniel Kavan[1, 2]; Jana Novakova[3]; Tibor Mosko[4]; Karel Holada[4]; Petr Pompach[5]; Petr Novak[1, 2]; Petr Man[1, 2]; *[1]Faculty of Science, Charles University, Prague, Czech Republic; [2]BioCeV – Institute of Microbiology, The Czech Academy of Sciences, Prague, Czech Republic; [3]AffiPro s.r.o, Vestec, Czech Republic; [4]Institute of Immunology and Microbiology, 1st Faculty of Medicine, Charles University, Prague, Czech Republic; [5]BioCev – Institute of Biotechnology, The Czech Academy of Sciences, Prague, Czech Republic*

MP 728 **Deep learning models combined to ultrafast DIA analysis enables rapid pathogen identification in urinary tract infections**; Florence Roux-Dalvai[1]; Antoine Lacombe-Rastoll[1]; Simon Pelletier[1]; Clarisse Gotti[1]; Mickaël Leclercq[1]; Ève Bérubé[2]; Marie-Ève Thibeault[1]; Maurice Boissinot[2]; Cristina C. Jacob[3]; Neloni R. Wijeratne[3]; Dorte B. Bekker-Jensen[4]; Nicolai Bache[4]; Maciej Bromirski[5]; Sandra Isabel[2]; Arnaud Droit[1]; *[1]AD Lab - Proteomics and Computational Biology laboratory, CHU de Québec - Université Laval Research Center, Québec, QC; [2]Infectiology Research Centre, CHU de Québec Université Laval Research Center, Québec, QC; [3]ThermoFisher Scientific, San Jose, CA; [4]Evosep, Odense, Denmark; [5]Thermo Fisher Scientific, Bremen, Germany*

MP 729 **Enhanced secretomics workflow reveals organ-dependent secreted protein landscape across multiple murine tissues**; Amanda L Smythers[1, 2]; Joao A. Paulo[1]; Melanie J Mittenbuhler[1, 2]; Katherine A Blackmore[1, 2]; Sumeet A Khetarpal[2, 3]; Bruce M Spiegelman[1, 2]; Steven P. Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Dana Farber Cancer Institute, Boston, USA, MA; [3]Massachusetts General Hospital, Harvard Medical School, Charlestown, MA*

MP 730 **Enhancing Sensitivity in Single-Cell Proteomics: Upgrading Triple Quadrupole Mass Spectrometer with S-Funnel Interface for Precise Quantitative Analysis**; Sehong Min[1]; Pearl Kwantwi-Barima[1]; Isaac K. Attah[1]; Thomas L. Fillmore[2]; Matthew J. Gaffrey[1]; William B. Chrisler[1]; Reta Birhanu Kitata[1]; Yehia M. Ibrahim[1]; Tujin Shi[1]; *[1]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [2]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA*

MP 731 **Ever Simpler: Streamlining Proteomics with S-Trap Turbo and BCA-No-More**; Stefan Loroch[1, 2]; Sandra Wilson[1]; Alexandre Zougman[3]; John P Wilson[1]; *[1]Protifi, LLC,* *Fairport, NY; [2]Ruhr-University Bochum, Bochum, Germany; [3]University of Leeds, Leeds, United Kingdom*

MP 732 **Highly multiplexed proximity labeling proteomics for spatiotemporal profiling of the suborganellar proteome**; Dong-Gi Jang[1, 2]; Sanghee Shin[1, 2]; Song-Yi Lee[3]; Yeon Choi[2]; Hyun-Woo Rhee[3]; Jong-Seo Kim[1, 2]; *[1]School of Biological Sciences, Seoul National University, Seoul, South Korea; [2]Center for RNA Research, Institute of Basic Science (IBS), Seoul, South Korea; [3]Department of Chemistry, Seoul National University, Seoul, South Korea*

MP 733 **Integrated sequencing of transcripts and proteins at the single molecule level to detect isoforms and proteotypic peptides in filament biomarkers**; Kenneth A. Skinner[1]; Natchanon Sittipongpittaya[2]; Gloria Sheynkman[2]; *[1]Quantum-Si Incorporated, Branford, CT; [2]University of Virginia, Charlottesville, VA*

MP 734 **Nanosecond infrared laser (NIRL) based tissue sampling enables spatially resolved proteomics for identification of region-specific metabolic processes in renal tissue**; Manuela Moritz[1]; Annika Gerdes[1]; Antonia Gocke[1]; Hartmut Schlüter[1]; Jan Hahn[1]; *[1]University Medical Center Hamburg-Eppendorf (UKE), Hamburg, Germany*

MP 735 **Protein cooking: gas phase separation of protein fragment ions generated by Thermal-CID**; Hieu Cuong Le[1]; Patrick Pribil[1]; Yves Le Blanc[2]; *[1]SCIEX, Concord, ON; [2]SCIEX, Concord, On, ON*

MP 736 **Proteomics method development for systems-wide protein turnover measurements in cynomolgus monkey**; Ghazaleh Yassaghi[1]; Vahid Farrokhi[1]; Hendrik Neubert[1]; *[1]Pfizer Inc., Andover, MA*

MP 737 **Reagent restoration using crosslinking chemistry improves BioID data quality**; Jonathan St-Germain[1]; Faith Au Yeung[2]; Vinitha Macwan[2]; Brian Raught[2]; *[1]Princess Margaret Cancer Centre, Toronto, ON; [2]Princess Margaret Cancer Centre, University Health Network, Toronto, ON*

MP 738 **Targeting the small proteome: Specialized methods for sequencing and the discovery of small proteins / sORFs in prokaryotes**; Jakob Meier-Credo[1]; Benjamin Heiniger[2]; Christian H. Ahrens[2]; Julian D. Langer[1, 3]; *[1]Max-Planck-Institute of Biophysics, Frankfurt, Germany; [2]Molecular Ecology, Agroscope & SIB Swiss Institute of Bioinformatics, Zurich, Switzerland; [3]Max Planck Institute for Brain Research, Frankfurt, Germany*

MP 739 **Throughput and the Plasma Proteome- How Olink and LCMS can Synergize Biomarker Discovery**; Jessica Moore[1]; Jaison Arivalagan[1]; Tiffany Louie[1]; Ray Clemens[1]; Leslie Wilkinson[1]; Ana Gil De Bona[1]; Danielle Gutierrez[1]; *[1]Discovery Life Sciences, Huntsville, AL*

MP 740 **Towards proteome analysis of single extracellular vesicles**; Ole Østergaard[1]; Pierre Sabatier[1, 2]; Charlotte Hjort[1]; Jesper Velgaard Olsen[1]; *[1]NNF CENTER FOR PROTEIN RESEARCH, Copenhagen, Denmark; [2]Department of Surgical Sciences, Uppsala University, Uppsala, Sweden*

MP 741 **A Novel Proteomics Magnetic Clean-up Bead for Automated Mass Spectrometry Sample Preparation**; Maowei Dou[1]; Suzanne Smith[1]; Erum Raja[1]; Leigh Foster[1]; Kevin Yang[2]; Amirmansoor Hakimi[2]; Kay Opperman[1]; Bhavin Patel[1]; Ryan Bomgarden[1]; *[1]Thermo Fisher Scientific, Rockford, Illinois; [2]Thermo Fisher Scientific, San Jose, CA*

MP 742 **Direct Identification of Intact Proteins Using a Low-Resolution Mass Spectrometer with CIDn/ETnoD**; Cheng-Yu Kuo[1]; Jie-Teng Toh[1]; Yi-Feng Zheng[1]; Wei-Chen Wang[1]; Han-ju Chien[2]; Chien-Chen Lai[1, 3, 4, 5, 6]; *[1]Institute of Molecular Biology, National Chung Hsing University, Taichung city, Taiwan; [2]Department of Biochemical Science and Technology, National Chiayi University, Chiayi city, Taiwan; [3]Advanced Plant Biotechnology Center, National Chung Hsing University, Taichung city, Taiwan; [4]Graduate Institute of Chinese Medical Science, China Medical University, Taichung city, Taiwan; [5]Ph.D. Program in Translational Medicine, National Chung Hsing University, Taichung, Taiwan; [6]Rong Hsing Research Center for Translational Medicine, National Chung Hsing University, Taichung, Taiwan*

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MP 743 **Studying the Proteome Heterogeneity of Naïve Human Pluripotent Stem Cells and Trophectoderm-like Cells Using Label-free Single-cell Proteomics**; Julia Bubis[1]; Harunobu Kagawa[2]; Manuel Matzinger[1]; Jana Slovakova[2]; Theresa M. Sommer[2]; Tabiwang N Arrey[3]; Eugen Damoc[3]; Peter Pichler[1]; Nicolas Rivron[2]; Karl Mechtler[1]; *[1]Research Institute of Molecular Pathology (IMP), Vienna BioCenter, Vienna, Austria; [2]Institute of Molecular Biotechnology (IMBA), Austrian Academy of Sciences, Vienna BioCenter (VBC), Vienna, Austria; [3]Thermo Fisher Scientific, Bremen, Germany*

MP 744 **Differential ion mobility on an Astral mass spectrometer provides new insights into thymocyte maturation**; Eric Bonneil[1]; Sylvie Brochu[1]; Lilian Heil[2]; Tonya Pekar-Hart[2]; Michael W. Belford[3]; Cornelia Boeser[3]; Jean-Jacques Dunyach[3]; Claude Perreault[4, 5]; Pierre Thibault[4, 6]; *[1]Universite de montreal, Montreal, QC; [2]Thermo Fisher Scientific, San Jose, CA; [3]ThermoFisher Scientific, San Jose, CA; [4]IRIC Université de Montréal, Montreal, QC; [5]Department of Medicine, Université. de Montréal, Montreal, QC; [6]Department Of Chemistry Université de Montréal, Montreal, QC*

MP 745 **Optimization of data-dependent acquisition settings for TMT-based single-cell proteome profiling**; Sachini N Moratuwage[1]; Kei Webber[1]; Xiaofeng Xie[1]; Siqi Huang[1]; Nathaniel Axtell[1]; Ryan T. Kelly[1]; *[1]Brigham Young University, Provo, UT*

MP 746 **MALDI-ICC and SpaceM on PBMCs Spiked with Cancer Cells for Highly Multiplexed, Multiomic and Multimodal Single-Cell Profiling**; Ziying Liu[1]; Gargey Yagnik[1]; Sharath K. Menon[2]; Shawn Owens[3]; Leonardo G. Dettori[1]; Philip Carvalho[1]; Kenneth J. Rothschild[1, 4]; Theodore Alexandrov[2, 3, 5]; Mark J. Lim[1]; *[1]AmberGen Inc., Billerica, MA; [2]Structural and Computational Biology Unit, European Molecular Biology Laboratory (EMBL), Heidelberg, Germany; [3]BioStudio, BioInnovation Institute, Copenhagen, Denmark; [4]Department of Physics and Photonics Center, Boston University, Boston, MA; [5]Molecular Medicine Partnership Unit, EMBL and Heidelberg University, Heidelberg, Germany*

MP 747 **scPiMS: a novel strategy for profiling intact proteoform signals from single cells**; Jared Kafader[1]; Pei Su[1]; Michael A. Hollas[1]; Stanislav Rubakhin[2]; Ryan T. Fellers[1]; Jonathan V Sweedler[2]; Neil L. Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]University of Illinois at Urbana-Champaign, Champaign, Illinois*

MP 748 **Robust, convenient, high throughput single cell proteomics**; Reta Birhanu Kitata[1]; Zhangyang Xu[1]; Rui Zhao[2]; Daniel J. Orton[1]; Nadia Bayou[3]; Mara Serena Serafini[3]; Thomas L. Fillmore[2]; William B. Chrisler[1]; Matthew J. Gaffrey[1]; Tao Liu[1]; Carolina Reduzzi[3]; Tujin Shi[1]; *[1]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [2]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; [3]Division of Hematology and Medical Oncology, Department of Medicine, Weill Cornell School of Medicine, New York, NY*

MP 749 **High-Throughput Single-Cell Metabolomics with SpaceM: High Reproducibility Enables Studying Multiple Cell Types**; Jeany Delafiori[1]; Shahraz Mohammed[1]; Andreas Eisenbarth[1]; Bishoy Wadie[1]; Bernhard Drotleff[1]; Mans Ekelof[1]; Alexander Mattausch[1]; Volker Hilsenstein[1]; Theodore Alexandrov[1]; *[1]EMBL, Heidelberg, Germany*

MP 750 **Statistical methods for handling cellular heterogeneity in quantitative scMS experiments: review simulations and recommendations**; Hannah Boekweg[1]; Devon Kohler[2]; Samuel H Payne[3]; Olga Vitek[2]; *[1]Brigham Young University,* *Provo, UT; [2]Northeastern University, Boston, MA; [3]BYU, Provo, UT*

MP 751 **Label-free capillary electrophoresis-mass spectrometry to sudy native N-glycome of single mammalian cells and ng-level blood isolates**; Anne-Lise Marie[1]; Yunfan Gao[1]; Alexander R. Ivanov[1]; *[1]Barnett Institute of Chemical and Biological Analysis, Dept. of Chemistry and Chemical Biology, Northeastern University, Boston, MA*

MP 752 **Label-free DIA-based workflow for single cell proteomic analysis using Evosep One and the Orbitrap Astral mass spectrometer**; Fernanda Salvato[1]; Min Huang[2]; Bernard Delanghe[3]; Kevin Yang[1]; Xiangjun Li[4]; Dorte-Bekker Jensen[5]; Nicolai Bache[5]; Tonya Pekar Hart[1]; Amirmansoor Hakimi[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]ThermoFisher Scientific, Shanghai, China; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Thermo Fisher Scientific, Shanghai, China; [5]Evosep, Odense, Denmark*

MP 753 **Label-free DIA-based workflow for single-cell proteomic analysis on an Orbitrap Exploris 480 mass spectrometer.**; Fernanda Salvato[1]; Bernard Delanghe[2]; Julia Kraegenbring[2]; David Hartlmayr[3]; Anjali Seth[3]; Tonya Pekar Hart[4]; Amirmansoor Hakimi[5]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific GmbH, Bremen, Germany; [3]Cellenion, Lyon, France; [4]Thermo Fisher Scientific – 355 River Oaks Pkwy, San Jose, California; [5]ThermoFisher Scientific, San Jose, CA*

MP 754 **Single Cell Fatty Acid Profiling with C=C Specificity using Multiple Reaction Monitoring(MRM)-profiling and Charge Switch Derivatization**; Pooja Saklani[1]; Caitlin Randolph[2]; Brianna Corman[3]; Gaurav Chopra[2, 4, 5, 6, 7, 8, 9]; *[1]Purdue University Department of Chemistry, West Lafayette, IN; [2]Purdue University, Department of Chemistry, West Lafayette, IN; [3]Department of Comparative Pathobiology, Purdue University, West Lafayette, IN; [4]Department of Computer Science (by courtesy), Purdue University, West Lafayette, IN; [5]Purdue Institute for Drug Discovery, West Lafayette, IN; [6]Regenstrief Center for Healthcare Engineering, West Lafayette, IN; [7]Purdue Institute for Cancer Research, West Lafayette, IN; [8]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; [9]Purdue Institute for Integrative Neuroscience, West Lafayette, IN*

MP 755 **Dynamics of single-cell protein covariation during epithelial–mesenchymal transition**; Saad Khan[1]; Rachel Conover[1]; Anand Asthagiri[1]; Nikolai Slavov[1, 2]; *[1]Northeastern University, Boston, MA; [2]Parallel Squared Technology Institute, Watertown, MA*

MP 756 **Increasing throughput while maintaining coverage depths in single cell proteomics using the timsTOF Ultra**; Christoph Krisp[1]; David Hartlmayr[2]; Anjali Seth[2]; Guilhem Tourniaire[2]; Taylor Skurnac[3]; Thorsten Ledertheil[1]; Jean-François Greisch[4]; Markus Lubeck[1]; Liling Fang[5]; *[1]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [2]Cellenion, Lyon, France; [3]Bruker Scientific, Billerica, MA; [4]Bruker Switzerland AG, Faellanden, Switzerland; [5]Bruker Scientific LLC, Billerica, MA*

MP 757 **Furthering Capabilities in Single Cell Metabolomics Using Single Cell Printing-Liquid Vortex Capture-Mass Spectrometry**; Stephen C Zambrzycki[1]; Vilmos Kertesz[1]; John F. Cahill[1]; *[1]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN*

MP 758 **A Microfluidic Platform for Extracellular Vesicle Sorting and Inline ESI-MS Analysis for Cell Therapy Biomanufacturing**; Gianna A Slusher[1]; Peter Kottke[1]; Andrei Fedorov[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

MP 759 **Single-cell MS lipid analysis: sample storage**; Stanislav Rubakhin[1, 2]; Jonathan V Sweedler[1, 2]; *[1]The Chemistry Department, University of Illinois at Urbana-Champaign, Urbana, IL; [2]Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, IL*

MP 760 **Tame Your Metabolomics Data Analysis with MeDUSA**; Laura A Hetzel[1]; Eric Hetzel[1]; Thomas Hankemeier[1]; Ahmed Ali[1]; *[1]Universiteit Leiden, Leiden, Netherlands*

MP 761 **Systematic evaluation of proteomics variation in label-free and multiplex single-cell proteomics workflows**; Ritin Sharma[1, 2]; Krystine Garcia-Mansfield[1, 2]; Brooke Lovell[1]; Rochelle Kofman[1]; Melissa N Martinez[1, 2]; Joshua Cantlon[3]; Andrew Leduc[4]; Patrick Pirrotte[1, 2]; *[1]Cancer and Cell Biology, Translational Genomics Research Institute, Phoenix, AZ; [2]Integrated Mass Spectrometry Shared Resource, City of Hope Comprehensive Cancer Center, Duarte, CA; [3]SCIENION US Inc., Phoenix, AZ; [4]Departments of Bioengineering, Biology, Chemistry and Chemical Biology, Single Cell Proteomics Center, and Barnett Institute, Northeastern University, Boston, MA*

MP 762 **Proteome asymmetry in mouse and human embryos before fate specification**; Aleksandra Petelski; *Parallel Squared Technology Institute, Watertown, MA*

MP 763 **Non-small cell Lung cancer single spheroid analysis using the cellenONE with proteoCHIP EVO 96 workflow on the timsTOF Ultra**; Christoph Krisp[1]; Verena Tellstroem[1]; David Hartlmayr[2]; Anjali Seth[2]; Guilhem Tourniaire[2]; Dorte Bekker-Jensen[3]; Nicolai Bache[3]; Markus Lubeck[1]; *[1]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [2]Cellenion, Lyon, France; [3]Evosep, Odense, Denmark*

MP 764 **Development of rapid and accurate cell picking and semi-automatic pretreatment system for single-cell proteomic and metabolomic analysis**; Kosuke Hata[1]; Masatomo Takahashi[1]; Mamoru Hirafuji[2]; Keisuke Nakata[1]; Kazuki Ikeda[1]; Maiko Goto[1]; Mie Uetsu[1]; Takeshi Bamba[1]; Yoshihiro Izumi[1]; *[1]Medical Institute of Bioregulation, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka-shi, Japan; [2]YODAKA Co., Ltd., 7-7 Shinkawasaki, Saiwai-ku, Kawasaki-shi, Japan*

MP 765 **Lie to me – The Importance of Knowing the Single Cell Proteomics Background**; Rupert Laurenz Mayer[1]; Julia A Bubis[1]; Manuel Matzinger[1]; Karl Mechtler[1, 2, 3]; *[1]Research Institute of Molecular Pathology (IMP), Vienna, Austria; [2]Institute of Molecular Biotechnology (IMBA), Vienna, Austria; [3]Gregor Mendel Institute of Molecular Plant Biology (GMI), Vienna, Austria*

MP 766 **Single-cell multi-omics analysis with Fucci3.2 cell cycle visualization probes**; Yoshihiro Izumi[1]; Kosuke Hata[1]; Asako Sawano[2]; Masatomo Takahashi[1]; Mamoru Hirafuji[3]; Kohta Nakatani[1]; Masaki Matsumoto[4]; Atsushi Miyawaki[2, 5]; Takeshi Bamba[1]; *[1]Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; [2]RIKEN Center for Brain Science, Waco, Japan; [3]YODAKA Co., Ltd,, Kawasaki, Japan; [4]Graduate School of Medical and Dental Sciences, Niigata University, Niigata, Japan; [5]RIKEN Center for Advanced Photonics, Wako, Japan*

MP 767 **Robust workflow for high-throughput quantitative analysis of low samples amounts and single-cells**; Tabiwang N. Arrey[1]; Santosh Renuse[2]; Jenny Ho[3]; Min Huang[4]; Shio Watanabe[5]; David Hartlmayr[6]; Anjali Seth[6]; Bernard Delanghe[7]; Nicolaie Eugen Damoc[7]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]ThermoFisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [4]Thermo Fisher Scientific, Shanghai, China; [5]Thermo Fisher Scientific, Yokohama, Japan; [6]Cellenion, Lyon, France; [7]Thermo Fisher Scientific, Bremen, Germany*

MP 768 **Ultra-high throughput workflow for robust and sensitive quantitative single cell analysis**; Bernard Delanghe[1]; Julia Kraegenbring[2]; Tabiwang Arrey[2]; Fernanda Salvato[3]; David Hartlmayr[4]; Anjali Seth[4]; Eugen Damoc[2]; Tonya Pekar Hart[3]; Thomas Moehring[2]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]ThermoFisher Scientific, San Jose, CA; [4]Cellenion, Lyon, France*

MP 769 **Exploring the Influence of the Number of Ions on Peptide Fragmentation Spectra**; Teeradon Phlairaharn[1]; Brian Searle[2]; *[1]Technical University of Munich (TUM), Freising, Germany; [2]Ohio State University, Columbus, OH*

MP 770 **Towards Preparation of 10k Single Cells Per Day for Tandem Mass Tag-based Single-cell Proteomics**; Ximena Sanchez-Avila[1]; H. Lavender Lin[1]; Tyler Hunter[1]; Kei Webber[1]; Xiaofeng Xie[1]; Ryan T. Kelly[1]; *[1]Brigham Young University, Provo, UT*

MP 771 **Enabling scalable single-cell proteomics by utilizing the unique analytical properties of the Evotip Pure**; Frederik Haugaard Vrdlovec Holck[1]; David Hartlmayr[2]; Anjali Seth[2]; Ole Hoerning[1]; Dorte B. Bekker-Jensen[1]; Nicolai Bache[1]; *[1]Evosep, Odense, Denmark; [2]Cellenion, Lyon, France*

MP 772 **Single-cell proteomic analysis of prostate cancer cell lines using a proteoCHIP-based TMT method**; Shimin Chen[1]; Vanessa Correll[1]; O. John Semmes[1]; Julius O. Nyalwidhe[1]; *[1]Eastern Virginia Medical School, Norfolk, VA*

MP 773 **Multicolumn low-flow nanoLC-MS platform for high-throughput label-free single-cell proteomics**; Chao Wang[1]; Siqi Huang[1]; Kei Webber[1]; Thy Truong[1, 2]; Xiaofeng Xie[1, 2]; Ryan T. Kelly[1]; *[1]Brigham Young University, Provo; [2]MicrOmics Technologies, Spanish Fork, UT*

MP 774 **Dissecting mammary stem cell heterogeneity in high-risk breast with a droplet-based low-input proteomic platform**; Matthew Waas[1]; Amanda Khoo[1, 2]; Pirashaanthy Tharmapalan[1]; Curtis W McCloskey[1]; Meinusha Govindarajan[1, 2]; Bowen Zhang[1, 2]; Shahbaz Khan[1]; Paul Waterhouse[1]; Rama Khokha[1, 2]; Thomas Kislinger[1, 2]; *[1]Princess Margaret Cancer Centre, University Health Network, Toronto, ON; [2]University of Toronto, Toronto, ON*

MP 775 **Deciphering Spatial Variation in Lipid Profiles of X-Ray Irradiated Cells using nLC and Obritrap 240 MS**; Rahul Ravi Deshpande[1]; Kyle D.G. Saunders[2]; Johanna Gerichten[2]; Bashar Amer[1]; Thomas Moehring[3]; Melanie Bailey[2]; Susan S Bird[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Department of Chemistry, University of Surrey, Guildford, United Kingdom; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 776 **Combining multiplexing with triggered MS/MS acquisition using super heavy TMT for targeted single cell proteomics**; Firdous A. Bhat[1]; Dong-Gi Mun[1]; Anu Jain[1]; Hiroshi Nishida[1]; Akhilesh Pandey[1]; *[1]Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, MN 55905, USA*

MP 777 **Untargeted single cell lipidomics using ion mobility spectrometry**; Seul Kee Byeon[1]; Jinyong Kim[1]; Dong-Gi Mun[1]; Erica Marie Forsberg[2]; Sven W Meyer[3]; Aiko Barsch[3]; Akhilesh Pandey[1]; *[1]Mayo Clinic, Rochester, MN; [2]Bruker Scientific, Billerica, MA; [3]Bruker Daltonics GmbH & Co. KG, Billerica, MA*

MP 778 **Towards spatially-resolved proteome mapping at single-cell resolution with laser ablation**; Liang Chen[1]; Yumi Kwon[1]; Andrey V. Liyu[1]; Julia Unsworth[2]; Lye Meng Markillie[1]; Dehong Hu[1]; Rashmi Kumar[1]; Sarah M. Williams[1]; Megan K. Ruhland[2]; Ying Zhu[3]; Ljiljana Paša-Tolić[1]; *[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99352, USA., Richland, WA; [2]Department of Cell, Developmental and Cancer Biology, Knight Cancer Institute, Oregon Health and Science University, Portland, Oregon; [3]Department of Microchemistry, Proteomics, Lipidomics and Next Generation Sequencing, Genentech, South San Francisco, CA*

MP 779 **Thermal Inkjetting Enabled Single-Cell Proteomics for Evaluating Outcomes of Genetic Manipulations and Tracking Bioengineered Proteins in Individual Cells**; Stanislau Stanisheuski[1]; Hyo Sang Jang[2]; Kavi Aashish Vaidya[1]; Alex Eddins[1]; Liping Yang[1]; Jeffrey Morre[1]; Claudia S. Maier[1]; *[1]Oregon State University, Corvallis, OR; [2]HP Inc, Corvallis, OR*

MP 780 **Deciphering Cellular Responses to Abiotic and Biotic Stress through Single-Cell Proteomics**; James M Fulcher[1]; Pranav Dawar[1]; Vimal Balasubramanian[2]; Tanya Winkler[2]; Sarah M Williams[2]; Amir Ahkami[2]; Ljiljana Paša-Tolić[2]; Ying Zhu[3]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Genentech Inc, South San Francisco, CA*

MP 781 **The Proteomics Landscape of PC12 Cells: Insights into Molecular Processes During Neuronal Differentiation and Maturation**; Arpa Ebrahimi[1]; Shuxin Chi[2]; Phoebe Lee[3]; Prongbaramee Colling[3]; Liping Yang[3]; Luke C Marney[3]; Leonard J Foster[2]; Claudia S. Maier[3]; *[1]OSU, Corvallis, OR; [2]University of British Columbia, Vancouver, BC; [3]Oregon State University, Corvallis*

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MP 782 **Standardizing retention times to reduce ambiguity of small molecule identification**; Huaxu Yu[1]; Tong Shen[1]; Jeremiah Wells[1]; Gert Wohlgemuth[1]; Uri Keshet[1]; Yendry Carvajal Miranda[1]; Yuanyue Li[1]; Oliver Fiehn[1]; *[1]West Coast Metabolomics Center, University of California, Davis, Davis, CA*

MP 783 **Understanding small aromatic systems fragmentation pathways of historic anthraquinone dyes from the Max Weaver Dye Library**; Morgan Demmler[1]; Nelson Vinueza[1, 2]; *[1]Wilson College of Textiles, NC State University, Raleigh, NC; [2]Department of Chemistry, NC State University, Raleigh, NC*

MP 784 **Optimization of AGC target value to Improve quantitation accuracy of trace-level analyte by orbitrap mass spectrometer**; Eric M Brown[1]; Jingyue Yang[1]; Tim Marzan[1]; Dan Berger[2]; Ee-Sunn Chia[2]; Obinna Ugwu-Oju[2]; Mohammad Mohiminul Islam[2]; Rachel Dunn[1]; Alicia Hoover[1]; *[1]Food and Drug Administration, St. Louis, MO; [2]Food and Drug Administration, Silver Spring, MD*

MP 785 **Impact of Mobile Phase Additive on APCI- and ESI-MS Ionization and In-Source Fragmentation of N-Nitrosamine Compounds**; Jessica N. Hoskins[1]; Monika Ladavicius[2]; John T. Lawler[1]; Richard A. Blessing[1]; Russell L. Hertzler[1]; *[1]AbbVie, North Chicago, IL; [2]University of Minnesota, Minneapolis, MN*

MP 786 **Development of an assay for atropine in rabbit plasma by LC/MS/MS and the impact of atropine esterase**; Jean-François Larocque[1]; Jeff Plomley[1]; Anahita Keyhani[1]; *[1]Altasciences, Laval, QC*

MP 787 **An LC-MS/MS method for bioanalysis of a molecular glue, pomalidomide, at sub-ng/mL levels in human plasma**; Eshani Galermo[1]; Ebru Selen[1]; Rahul Baghla[1]; *[1]SCIEX, Redwood City, CA*

MP 788 **RECENT AUSTRALIAN FLAVOUR RESTRICTIONS: ANALYSING THE CHEMICAL PROFILES OF “TOBACCO” AND “MINT” ELECTRONIC CIGARETTES**; Caitlin Jenkins[1, 2]; Jody Morgan[1, 2]; Celine Kelso[1, 2]; *[1]School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; [2]Molecular Horizons, University of Wollongong, Wollongong, Australia*

MP 789 **Chip-Based CE-MS Analysis of Serotonin in the Rodent Fetus During Early Brain Development – the Placental-Brain-Axis**; Chen Huang[1]; Jessica Kincade[2]; Cheryl S. Rosenfeld[2]; R. Michael Roberts[2]; Jonathan Sweedler[1]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL; [2]University of Missouri-Columbia, Columbia, MO*

MP 790 **A Sensitive and Robust Assay for Simultaneous Quantification of Methylprednisolone Acetate and Methylprednisolone in Human Plasma Treated with Sodium Fluoride**; Molly McBride[1]; Charlie Zha[2]; Natasha Morgan[1]; Aihua Liu[1]; *[1]Resolian (Formally Alliance Pharma), Malvern, PA; [2]Brii Biosciences, Durham, NC*

MP 791 **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[1]; Robert Huang[2]; Limin Chu[1]; Mo Xu[2]; Min Meng[1]; Guitao Wang[2]; Yuehui Ma[1]; Fan Pan[2]; Aining Li[2]; Aihua Liu[1]; *[1]Resolian (Formally Alliance Pharma), Malvern, PA; [2]Coherent Biopharma, Hefei, China*

MP 792 **Enantiomer differentiation using magnesium adduct complexes and tandem mass spectrometry: towards chiral recognition in metabolomics analyses**; Chenqin Cao[1]; Sandra Alves[2]; Jean-Claude Tabet[1, 2]; François Fenaille[1]; Christophe Junot[1]; Annelaure DAMONT[1]; *[1]Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), MetaboHUB, Gif-sur-yvette, France; [2]Faculté des Sciences et de l'Ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Sorbonne Université, Paris, France*

MP 793 **A Novel Assay to Measure Intracellular Endogenous Nucleotides and Active Antiretroviral Nucleotide Metabolites in Cell Lysate by LC-MS/MS**; Amanda P Schauer[1]; Craig Sykes[1]; Mackenzie L Cottrell[1]; Angela DM Kashuba[1]; *[1]University of North Carolina, Chapel Hill, NC*

MP 794 **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[1]; Stane Pajk[1]; Ema Valentina Brovč[2]; Tinkara Lekić[2]; *[1]University of Ljubljana, Faculty of Pharmacy, Ljubljana, Slovenia; [2]Novartis Pharmaceutical Manufacturing LLC, Menges, Slovenia*

MP 795 **Determination of Nitrosamine Impurities and NDSRI in Anti-diabetic Drugs on Shimadzu LCMS-8060NX**; Shao Hua Chia[1]; Siew Qi Yap[1]; Zhi Wei Edwin Ting[1]; *[1]Shimadzu (Asia Pacific), Singapore, Singapore*

MP 796 **LC-MS Method for the Detection and Quantitation of Fermentation End-Products in Spent Media**; Erin R. Tiede[1]; Dam Soh[2]; Patricia I. Diaz[2]; Valerie Frerichs[1]; *[1]Chemistry Instrument Center, Department of Chemistry, University at Buffalo, State University of New York, Buffalo, NY; [2]Department of Oral Biology, School of Dental Medicine, University at Buffalo, State University of New York, Buffalo, NY*

MP 797 **LC-QTOF Profiling of N-acyl-Homoserine Lactones Produced by Chromobacterium spp.**; Luer Wang[1]; Remy Kargodorian[1]; Alisha Harrison[2]; Scott Soby[2]; Charles A. Veltri[3]; *[1]Midwestern University College of Dental Medicine, Glendale, Arizona; [2]Midwestern University College of Biomedical Sciences, Glendale, Arizona; [3]Midwestern University College of Pharmacy-Glendale, Glendale, AZ*

MP 798 **Comparison of Exhaled Breath Condensate Markers Using Two Ionization Methods: Electrospray Ionization and Dielectric Barrier Discharge Ionization**; Tatiana Rodriguez[1]; Lia Ficaro[2]; Drew R Jones[2]; Rebecca Jones[2]; *[1]NYU Langone, Long Island City, NY; [2]NYU Langone, New York, NY*

MP 799 **Bioanalysis of lipid nanoparticle compounds in mouse and monkey plasma using LC-MS/MS**; Changyu Quang[1]; Joelle Lucarell[1]; Brad Bessette[1]; Samuel Brown[1]; Morgan Trimmer[1]; Maryam Goudarzi[1]; Liam Moran[1]; Dhananjaya Nayak[2]; Sushimit Maitra[3]; *[1]Charles River, Ashland, OH; [2]Charles River Laboratories, Worcester, MA; [3]Orna Therapeutics, Watertown, Massachusetts*

MP 800 **Enhancing Short-Chain Fatty Acids Quantification via GC-MS: Precipitation of Bromine Ions**; Cristina Arciniega[1]; Brandie M. Ehrmann[1]; *[1]The University of North Carolina at Chapel Hill, Chapel Hill, NC*

MP 801 **Fragmentation and Ionization Behavior of Synthetic, Anthraquinone Disperse Dyes**; Zoe J Millbern[1]; Nelson R Vinueza[1]; *[1]NC State University, Raleigh, NC*

MP 802 **Overcoming Challenges: Bioanalytical Support for Incurred Sample Reanalysis Failure during LC-MS/MS Analysis of Human Plasma Samples in Phase I Study**; Komal Kothari[1]; Ryan Johnson[1]; Xiaorong Liang[1]; Brian Dean[1]; Michael Van Parys[2]; *[1]Genentech Inc, South San Francisco, CA; [2]Labcorp Bioanalytical Services LLC, Indianapolis, IN*

MP 803 **Fast Isocratic LC/MS Orbitrap Method for the Simultaneous Quantitation of Uridine and Pseudouridine in Biological Samples**; Pradnya Patil[1]; Ling Fu[2]; Daniel Röth[1]; Yingfeng Deng[2]; Markus Kalkum[1]; *[1]City of Hope, Beckman Research Institute. Department of Immunology and Theranostics, Duarte, CA; [2]City of Hope, Beckman Research Institute, Department of Diabetes and Cancer Metabolism, Duarte, CA*

MP 804 **Highly Sensitive and Selective Method for Estimation of Formoterol at Sub-pg/mL in Human Plasma Using Shimadzu LCMS-8060NX**; Avinash B Gaikwad[1]; Chaitanya Krishna Atmakuri[1]; Yogesh G Arote[1]; *[1]ADC-Shimadzu Analytical India Pvt Ltd, NAVI MUMBAI, India*

VIRUSES AND VIRUS-LIKE PARTICLES

805-822

MP 805 **LC-MS based Peptide Mapping Methods for Characterization of Gene Therapy Vector Proteins**; Yu Zhou[1]; Derek Langeslay; *[1]Novartis, San Diego, CA*

MP 806 **Detection and relative quantitation of host cell proteins in lentivirus preparations**; Sahana Mollah[1]; Remco Van Soest[1]; Alicia Powers[2]; Chao-Xuan Zhang[2]; Timothy Lockey[2]; *[1]SCIEX, Redwood City, CA; [2]St.Jude Children's Research Hospital, Memphis, TN*

MP 807 **Recombinant Extracellular Vesicles as Tools for Membrane Protein Interactomics**; Shengya Cao[1]; Sean M Peterson[1]; Soren Muller[1]; Mike Reichelt[1]; Christian McRoberts Amador[2]; Nadia Martinez-Martin[1]; *[1]Genentech Inc, South San Francisco, CA; [2]Duke University, Durham, NC*

MP 808 **Comparison of the Empty/Full ratio assessment by Direct Mass Technology, Analytical Ultracentrifugation and Mass Photometry for AAV vectors**; Ryoji Nakatsuka[1, 2, 3]; Yuki Yamaguchi[1]; Tatsuya Aisu[1]; Kiichi Hiirohata[1]; Saki Shimojo[1]; Aoba Matsushita[1]; Yasuo Tsunaka[1]; Mitsuko Fukuhara[1, 4]; Tetsuo Torisu[1]; Susumu Uchiyama[1]; *[1]Osaka university, Osaka, Japan; [2]Shimadzu Corporation, Nakagyo-ku, Japan; [3]Osaka University Shimadzu Analytical Innovation Resarch Laboratories, Suita-shi, Japan; [4]U-Medico Inc, Suita-shi, Japan*

MP 809 **Tracking host cell protein (HCP) clearance on adeno-associated virus (AAV) products generated using HEK and Sf9 production systems**; Josh Smith[1]; Aaron Richardson[1]; Sara Carillo[1]; Marina Ainciburu[1]; Ioanna Tzani[1]; Michelle Chain[1]; Colin Clarke[1, 2]; Eugen Damoc[3]; Jonathan Bones[1, 2]; *[1]The National Institute for Bioprocessing Research & Training, Dublin, Ireland; [2]School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 810 **A combination of lectin-based fractionation and LC-MS/MS for glycosylation analysis of recombinant adeno-associated virus**; Yuki Yamaguchi[1]; Kentaro Ishii[1]; Sachiko Koizumi[2, 3]; Hiroaki Sakaue[4]; Takahiro Maruno[1, 5]; Mitsuko Fukuhara[1, 5]; Risa Shibuya[1]; Yasuo Tsunaka[1]; Aoba Matsushita[1]; Karin Bandoh[1]; Tetsuo Torisu[1]; Chie Murata-Kishimoto[2]; Azusa Tomioka[4]; Saho Mizukado[4]; Hiroyuki Kaji[6]; Yuji Kashiwakura[7]; Tsukasa Ohmori[7]; Atsushi Kuno[4]; Susumu Uchiyama[1]; *[1]Osaka University, Suita, Japan; [2]GlycoTechnica Ltd., Yokohama, Japan; [3]Precision System Science Co. Ltd., Matsudo, Japan; [4]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; [5]U-Medico Inc., Suita, Japan; [6]Nagoya University, Nagoya, Japan; [7]Jichi Medical University, Shimotsuke, Japan*

MP 811 **Key Applications of ELIT CDMS**; Rebecca J. D'Esposito[1]; Anisha Haris[2]; David Bruton[2]; Kevin Giles[2]; Keith G Richardson[2]; Chris Wheeldon[2]; Alistair Schofield[2]; David Eatough[2]; Ying Qing Yu[1]; Steve Preece[2]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom*

MP 812 **Optimizing Mass Spectrometer Conditions to Accurately Determine Full/Empty AAV Ratios: A Sample Half-Full Approach**; Kyle Patrick Bowen[1]; Michael Goodwin[1]; Michael W Senko[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 813 **Characterization of Adeno-Associated Virus (AAV9) Capsid Proteoforms using Multiple Ion Activations on an Orbitrap Tribrid Instrument**; Rafael D Donadelli Melani[1]; Kristina Srzentić[2]; Jingjing Huang[1]; Jake T Kline[3]; Christopher Mullen[1]; Luca Fornelli[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Reinach, Switzerland; [3]University of Oklahoma, Norman, OK*

MP 814 **Characterisation of Adeno Associated Virus Capsid Proteins using Top-Down LC-MS/MS**; Felipe Guapo[1]; Corentin Beaumal[1]; Josh Smith[1]; Silvia Millan Martin[1]; Sara Carillo[1]; Jonathan Bones[1, 2]; *[1]The National Institute for Bioprocessing Research & Training, Dublin, Ireland; [2]School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland*

MP 815 **Mass Spectrometry based characterization and identification of an N-terminal acetylated viral capsid protein 2 in Adeno-associated virus capsid proteins**; Ruiyi Dong[1]; Dingyi Wen[1]; Malgorzata Szyjka[1]; Xiaofeng Yang[1]; Paul Weinreb[1]; *[1]Biogen, Biologics Drug Discovery, Cambridge, MA*

MP 816 **Optimization of Adeno-Associated Virus peptide mapping using trapped ion mobility spectrometry**; Isin T Sakallioglu[1]; Anjali Alving[1]; Guillaume Tremintin[2]; *[1]Bruker Scientific, LLC, Billerica, MA; [2]Bruker Scientific LLC, San Jose, CA*

MP 817 **Automated Quantitation of Adeno-Associated Virus Byproducts Using Individual Ion Mass Spectrometry**; Ryan T. Fellers[1, 2]; Michael A. R. Hollas[1]; Bryan P. Early[1]; Joseph B. Greer[1, 2]; Kenneth R. Durbin[2]; Mike Goodwin[3]; Ping Yip[3]; Kristina Srzentic[3]; Kyle P. Bowen[3]; Michael W. Senko[3]; Samuel E Janisse[1]; Jared Kafader[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Proteinaceous, Inc., Evanston, IL; [3]Thermo Fisher Scientific – 355 River Oaks Pkwy, San Jose, California*

MP 818 **Profiling HIV-1 Virion Complexity at the Proteoform Level**; Claire E Boos[1]; Mark Scalf[1]; James W Bruce[2, 3]; Rachel M Miller[1]; Nathan M Sherer[2, 3]; Lloyd M Smith[1]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [2]McArdle Laboratory for Cancer Research, University of Wisconsin-Madison, Madison, WI; [3]Institute for Molecular Virology, Madison, WI*

MP 819 **The metabolic basis of dengue virus NS1-induced vascular leak in mouse tissues**; Paul S Soma[1]; Jaime Cardona-Ospina[2]; Barbara Graham[1]; Hannah Laurence[1]; Scott B Biering[2]; Eva Harris[2]; Rushika Perera[1]; *[1]Department of Microbiology, Immunology and Pathology, Center for Metabolism of Infectious Diseases, Colorado State University, Fort Collins, Colorado; [2]Division of Infectious Diseases and Vaccinology, School of Public Health, University of California, Berkeley, Berkeley, California*

MP 820 **Huge and Heterogeneous: Probing Biophysical Properties of Lipid Nanoparticles and Viruses with Charge Detection Mass Spectrometry**; Zachary M Miller[1]; Li F Lin[1]; David V Schaffer[1]; Justin W Torpey[2]; Lokesh Narsineni[2]; Yue-xuan Li[2]; Matthew R Gardner[2]; Evan R Williams[1]; *[1]University of California, Berkeley, Berkeley, CA; [2]Scribe Therapeutics, Alameda, CA*

MP 821 **Characterization of Bacteriophage P22 Procapsid and Wiffle Ball Structures by Charge Detection Mass Spectrometry**; Luke W Hawkins[1]; Isaiah R Moss[1]; Shelby M Klein[1]; Martin F Jarrold[1]; *[1]Indiana University Bloomington, Bloomington, IN*

MP 822 **Enabling icIEF Peak Identification: AAV Capsid Protein Fractionation on MauriceFlex and Subsequent Analysis by LC-MS**; Xiaoping He[1]; Sisi Huang[1]; Will McElroy[2]; Melissa Anderson[1]; Courtney Sloan[1]; Thomas Powers[1]; Chris Heger[2]; Tom Lerch[1]; *[1]Pfizer Inc, Chesterfield, MO; [2]ProteinSimple, Bio-Techne, San Jose, CA*

TUESDAY POSTERS

Set up all Tuesday posters
7:00 - 8:00 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
7:00 - 8:00 pm

AMBIENT IONIZATION: APPLICATIONS II
001-021

TP 001 **Origins of Reaction Acceleration and Unusual Reactions in Charged Droplets**; Casey J Chen[1]; Evan R Williams[1]; *[1]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[1]; Ching Kao[2]; Ming-Yang Wang[3]; Cheng-Chih Hsu[1, 4]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]Department of Medical Oncology, National Taiwan University Cancer Center, Taipei, Taiwan; [3]Department of Surgical Oncology, National Taiwan University Cancer Center, Taipei, Taiwan; [4]Leeuwenhoek Laboratories, Co. Ltd., Taipei, Taiwan*

TP 003 **Direct Dual Polarity Mass Spectrometry Imaging (DDPMSI) of Renal Cell Carcinoma**; Rachel Wood[1]; Malek Hassan[1]; Rachel L. Theriault[2]; Randy E. Ellis[2, 3]; Kevin Ren[4]; Richard D. Oleschuk[1]; *[1]Department of Chemistry, Queen's University, Kingston, ON; [2]School of Computing, Queen's University, Kingston, ON; [3]Department of Surgery, Queen's University, Kingston, ON; [4]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[1, 2]; Nicolás M. Morato[2]; R. Graham Cooks[2]; *[1]Indiana University Indianapolis, Indianapolis, IN; [2]Purdue University, West Lafayette, IN*

TP 005 **Development of rapid screening methods for herbs used in Traditional Chinese Medicine (TCM)**; TIANHUI YU[1]; James Reynolds[1]; *[1]Loughborough University, Loughborough, United Kingdom*

TP 006 **Automated Laser Assisted-Rapid Evaporative Ionisation Mass Spectrometry (LA-REIMS) for cell line phenotype predication 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[1, 2]; Chi-Yang Lee[2]; Jia-Cheng Chen[2]; Rui-Ying Hong[2]; Chun-Hsiu Chiu[2]; Hye Hyun Yoo[1]; Jentaie Shiea[2]; *[1]College of Pharmacy, Hanyang University, Ansan, South Korea; [2]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[1]; Jitka Konvalinkova[1]; Jan Bucek[2]; Magdalena Vagnerova[1]; Vladimir Vrkoslav[3]; David Sykora[1]; Martin Kuchar[1]; Josef Cvacka[3]; Michael Volny[1, 4]; *[1]University of Chemistry and Technology Prague, Prague 6 - Dejvice, Czech Republic; [2]Plasmion GmbH, Augsburg, Germany; [3]Institute of Organic Chemistry and Biochemistry of the CAS, Prague 6 - Dejvice, Czech Republic; [4]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 Iqfath[1]; Manxi Yang[1]; Julia Laskin[1]; *[1]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[1]; Myles Q. Edwards[1]; R. Graham Cooks[1]; *[1]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[1]; Kaitlyn Loomas[1]; Yifei Wang[2]; Dale Woerner[1]; Benjamin Bohrer[2]; Tyson Brown[3]; Heather Bruce[4]; Marcio Duarte[5]; Jerrad Legako[1]; *[1]Texas Tech University, Lubbock, Texas; [2]The Ohio State University, Columbus, OH; [3]Cargill Meat Solutions, Wichita, Kansas; [4]University of Alberta, Edmonton, AB; [5]University of Guelph, Guelph, ON*

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[1]; Ayoung Kim[1]; Matthew A. Turner[1]; Paul F. Kelly[1]; *[1]Loughborough University, Loughborough, United Kingdom*

TP 013 **Online ultrafast trypsin digestion of LC-separated proteins using microdroplet digestion**; Praneeth Ivan Joel FNU[1]; Timothy Yaroshuk[1]; Md Tanim-Al Hassan[1]; Harsha Gunawardena[2]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]JOHNSON AND JOHNSON, Spring House, PA*

TP 014 **Identification of Carpaine in Carica papaya Leaf Products using Direct Analysis in Real Time Mass Spectrometry (DART-MS)**; Piyawadi Khaoiam[1]; Patanachai Limpikirati[1, 2]; Rossarin Tansawat[1, 2]; *[1]Department of Food and Pharmaceutical Chemistry, Faculty of Pharmaceutical Sciences, Chulalongkorn University, Bangkok, Thailand; [2]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[1]; John Dane[1]; Kirk Jensen[1]; Bryan Katzenmeyer[1]; *[1]JEOL USA, Inc., Peabody, MA*

TP 016 **Exploring the capability of the Waters™ RADIAN™ ASAP mass spectrometer for simple, rapid detection of antimicrobials in food and feed**; Annette O Farrell[1]; Panagiotis Manesiotis[1]; Simon Cameron[1]; *[1]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[1]; Michael Woolman[2]; Francis Talbot[1]; Alexa Fiorante[2]; Yuki Sata[3]; Hiroyuki Ogawa[3]; Fumi Yokote[3]; Nicholas Bernards[3]; Michael Cabanero[3]; Nhu-An Pham[1]; Nikolina Radulovich[1]; Benjamin Lok[1]; Kazuhiro Yasufuku[3]; Ming-Sound Tsao[1]; Howard Ginsberg[4]; Arash Zarrine-Afsar[5]; *[1]Princess Margaret Cancer Centre, University Health Network, Toronto, ON; [2]Department of Medical Biophysics, University of Toronto, Toronto, ON; [3]University Health Network, Toronto, Ontario; [4]Unity Health Toronto, St Michael's Hospital, Toronto, Ontario; [5]University of Toronto, Toronto, ON*

TP 018 **DPiMS-MS (PESI) combined with vacuum differential mobility spectrometry for rapid clinical/forensic analysis**; Gordon C Kearney[1]; Patrick Knight[1]; Andrew Entwistle[1]; Franck SAINT-MARCOUX[2]; Pauline GRIFFEUILLE[2]; Souleiman EL BALKHI[2]; Ann-Christin Ann-Christin Niehoff[3]; Stephane Moreau[3]; *[1]Shimadzu Research Laboratory (Europe) Ltd., Manchester, United Kingdom; [2]University Hospital of Limoges, Limoges, France; [3]Shimadzu Europa GmbH, Duisburg, Germany*

TP 019 **Advanced Paper Spray Ionization Mass Spectrometry: TargetedPolyamine Odor MoleculesAnalysisbyAldehyde-Functionalized Cellulose Filter Paper**; Egodage Udeesha Inoshi De Silva[1]; Jianchuan Wen[1]; Yuyu Sun[1]; Anyin Li[2]; Pengyuan Liu[1]; *[1]University of Massachusetts, Lowell, Lowell, MA; [2]University of New Hampshire, Durham, NH*

TP 020 **GC-SICRIT-MS for Rapid Chemical Analysis of Electronic Cigarette Liquid**; Xiaoqing Wang[1]; Xiaokun Duan[1]; Charles C. Liu[1]; *[1]ASPEC Technologies, Suzhou, China*

TP 021 **Rapid Quantitative Screening of 18 Synthetic Cannabinoids in Urine Using DART-MS Analysis**; Terry L Bates[1]; William Fatigante[2]; Alex Maggitti[3]; Francois Espourteille[2]; *[1]Bruker Scientific, Billerica, MA; [2]Bruker Scientific, LLC, Billerica, MA; [3]DrugScan, Inc., Horsham, PA*

BIOMARKERS: QUANTITATIVE ANALYSIS I
022-048

TP 022 **Proteomic multi-marker model for diagnosis of obsessive compulsive disorder by multiple reaction monitoring-mass spectrometry**; Yeongshin Kim[1]; Dongyoon Shin[2]; Junho Park[2, 3]; Chun Il Park[4]; Se Joo Kim[5]; Youngsoo Kim[1, 2]; *[1]Department of Medical Science, School of Medicine, CHA University, Pangyo, South Korea; [2]Proteomics Research Team, CHA Institute of Future Medicine, Pangyo, South Korea; [3]Department of Pharmacology, School of Medicine, CHA University, Pangyo, South Korea; [4]Department of Psychiatry, CHA Bundang Medical Center, CHA University, Pangyo, South Korea; [5]Department of Psychiatry, Yonsei University College of Medicine, South Korea*

TP 023 **Bile proteomics for identifying biomarkers to differentiate hepatobiliary diseases**; Hyunesoo Kwon[1]; Young Eun Kim[2, 3]; Pham Ha Chau[2, 4]; Hoeil Chung[5]; Dukjin Kang[2]; Tae-Young Kim[1]; *[1]School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea; [2]Korea Research Institute of Standards and Science, Daejeon, South Korea; [3]Gwangju Institute of Science and Technology, Gwangju, South Korea; [4]Chungnam National University, Daejeon, South Korea; [5]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[1]; Angela Lu[1]; Long Yuan[1]; *[1]Biogen, Cambridge, MA*

TP 025 **prmPASEF HT: High sensitivity and throughput for absolute quantitation of plasma proteins**; Simonas Savickas[1]; Sebastian Mueller[1]; Véronique Laforte[1]; Tejas Gandhi[1]; Roland Bruderer[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

TP 026 **Improving Measurement Traceability in Untargeted Metabolomics: A Key to Cross-Study Comparisons**; Andre Märtens[1, 2]; Karsten Hiller[2]; Gavin O'Connor[1, 2]; *[1]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany; [2]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[1]; Jonathan Rochon[1]; Sarah Demers[1]; Serge Auger[1]; Jean Lacoursière[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC*

TP 028 **Quantitative estimation of urine proteins for biomarker discovery by Data-independent acquisition mass spectrometry (DIA-MS)**; Tadashi Yamamoto[1]; Keiko Yamamoto[1]; *[1]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 MoltIIIb cells**; Bao-Jen Shyong[1]; Matthew T. Mazur[2]; Guoxin Wu[3]; Brian C. Magliaro[3]; Weixun Wang[1]; *[1]PDMB, MRL, Merck & Co., Inc., West Point, PA; [2]PDMB, MRL, Merck & Co., Inc., West Point,, PA; [3]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[1]; Tai-Tu Lin[1]; Soumyadeep Sarkar[1]; Adam C Swensen[1]; Athena M Schepmoes[1]; Thomas L. Fillmore[1]; James P Delany[2]; Bret H Goodpaster[2]; Tujin Shi[1]; Wei-Jun Qian[1]; Jon M. Jacobs[1]; A2CPS Consortium[3]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]AdventHealth Research Institute, Orlando, FL; [3]NIH Commonfund, Bethesda, MD*

TP 032 **Quantitative Assay for Diacylglycerol Kinase Kappa with Mass Spectrometry and Parallel Reaction Monitoring**; Oktay CAKIL[1]; Anastasiia PETROVA[1]; Luc NEGRONI[1]; Hervé MOINE[1]; *[1]Université de Strasbourg, CNRS, Inserm, IGBMC UMR 7104- UMR-S 1258, F-67400 Illkirch, France, ILLKIRCH, France*

TP 033 **Comparing triple quadrupole mass spectrometry platforms for quantifying Alzheimer's disease biomarker peptides in cerebrospinal fluid**; Grayson Goss[1]; Morgan Elmor[1]; Allan I. Levey[1]; James J. Lah[1]; Blaine R. Roberts[1]; Nicholas T. Seyfried[1]; Caroline M. Watson[1]; [1]*Emory University School of Medicine, Atlanta, GA*

TP 034 **A sensitive determination of bisphenol A and its 11 analogs and triclosan in urine by UPLC-MS/MS**; Eric Gaudreau[1]; Sébastien Gagné[1]; Patrick Bélanger[1]; Normand Fleury[1]; [1]*Centre de Toxicologie du Québec (CTQ/INSPQ), Québec, QC*

TP 035 **Systematic Evaluation of Proteomic Responses Related to Multisystem Proteinopathy 1 using iPSC-derived Cerebral Organoids**; Feng Wang[1]; Shan Li[1]; Baiyi Quan[2]; Tsui-Fen Chou[1, 2]; [1]*Division of Biology and Biological Engineering, California Institute of Technology, Pasadena, CA;* [2]*Proteome Exploration Laboratory, Beckman Institute, California Institute of Technology, Pasadena, CA*

TP 036 **Towards Comprehensive Plasma Proteomics: Optimizing PRM-PASEF for Disease Biomarker Discovery**; Raghothama Chaerkady[1]; Morgan Fair[1]; Liang Zhao[1]; Qing Wang[1]; [1]*CompleteOmics, Halethorpe, MD*

TP 037 **Unveiling Real-time Changes: In Vivo Solid Phase Microextraction of Ultra-Trace Endogenous Psychedelics**; Min Liu[1, 2]; Oliver Fiehn[1, 2]; David E. Olson[2, 3, 4, 5]; Cassandra Hatzipantelis[2, 3, 4, 5]; Yara Ahmad Khatib[3]; [1]*West Coast Metabolomics Center, University of California Davis, Davis, CA;* [2]*Institute for Psychedelics and Neurotherapeutics, University of California, Davis, Davis, California;* [3]*Department of Chemistry, University of California, Davis, Davis, California;* [4]*Department of Biochemistry and Molecular Medicine, School of Medicine, University of California, Davis, Sacramento, California;* [5]*Center for Neuroscience, University of California, Davis, Davis, California*

TP 038 **Development of On-line Solid Phase Extraction LC/MS/MS Method for Quantification of 30 Bile Acids in Feces**; Amanda Blake[1]; Gabrielle Sakel[1]; Madison Perez[1]; Jake Chaconas[1]; Jan Suchodolski[1]; [1]*Gastrointestinal Lab, Texas A&M University, College Station, TX*

TP 039 **A High-Throughput, In-Depth Investigation into the Immunological Effects of Lipopolysaccharide Challenged Mice in Neat Plasma on Orbitrap Astral Mass Spectrometer**; Jana Richter[1]; Nicolas Hartel[1]; Kevin Yang[1]; Amirmansoor Hakimi[1]; Stephanie Samra[1]; [1]*Thermo Fisher Scientific, San Jose, CA*

TP 040 **Optimization of mass spectrometry methods for longitudinal measurement of biomarkers in Duchenne muscular dystrophy**; Ahmed Naveed[1]; Yubin Ki[1]; Elissa Recinos[1]; Dexter Chow[1]; Emily Canessa[1]; Yetrib Hathout[1]; [1]*Binghamton University-SUNY, Binghamton, NY*

TP 041 **Multi-Omics for Plasma: A Three-in-One End-to-End Automated Sample Preparation and LC/MS Metabolomics, Lipidomics, and Proteomics Workflow**; Christian Klein[1]; Karen E Yannell[1]; Cate Simmermaker[1]; Sierra D. Durham[1]; Genevieve Van De Bittner[1]; Mark Sartain[1]; Sheher Banu Mohsin[1]; Linfeng Wu[1]; [1]*Agilent Technologies, Santa Clara, CA*

TP 042 **Seasonal variation of neonicotinoids and their metabolites in Iowa surface and groundwaters**; Wenjing Xi; *Center for Health Effects of Environmental Contamination at the University of Iowa, Iowa City, Iowa*

TP 043 **Hydrophilic Interaction Liquid Chromatography Mass Spectrometry Enables Cellular Assay Development to Identify Inhibitors of Glycine N-Methyltransferase**; Jonathan Shrimp[1]; Quinlin Hanson[1]; Nate Hoxie[1]; John Janiszewski[1]; Vinoth Chenniappan[1]; Colin Kelly[1]; Min Shen[1]; Samarjit Patnaik[1]; Matthew D Hall[1]; [1]*NCATS/NIH, Rockville, MD*

TP 044 **High-throughput Quantification of 802 Peptides in Blood Plasma using 6495D Triple Quadrupole and Evosep One**; Hoi-Ting Wu Quanrud[1]; Linfeng Wu[2]; Hao Qian[1]; Yanan Yang[2]; Benjamin Ta[1]; Jessica Chan[1]; Purva Ranjan[1]; Robert Zawada[1]; Philip Ma[1]; Yi (JIMMY) Zeng[1]; Bruce Wilcox[1]; [1]*PrognomiQ Inc, San Mateo, CA;* [2]*Agilent Technologies, Santa Clara, CA*

TP 045 **Analysis of 3-Hydroxymyristic acid by LC-MS/MS in plasma samples of rats dosed with endotoxin**; Usha Mishra; *University of Minnesota, Minneapolis Mn, MN*

TP 046 **A Simple and Sensitive LC-MS/MS Method for Quantification of 7α-hydroxy-4-cholesten-3-one (C4) in Human Serum**; Aiping Zhu[1]; Tian-Sheng Lu[1]; Shuyu Hou[1]; [1]*Medpace, Cincinnati, OH*

TP 047 **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[1, 2]; Fangteng Dai[1, 2]; Jacki Jacki Rorabaugh[1, 3]; Juline Bryson[1, 4]; Hussein Hallak[1, 5]; Thelma Angeles[1, 2]; [1]*Teva Pharmaceuticals, West Chester, PA;* [2]*Biomarker and Metabolism Analytics, West Chester, PA;* [3]*Translational Medicine, West Chester, PA;* [4]*Clinical Development, West Chester, PA;* [5]*DMPK, Netanya, Israel*

TP 048 **Sensitive Detection and Quantitation of Protein Components of the Complement Pathway**; Luis F Schachner[1]; Cong Wu[1]; Jianhui Zhu[2]; Tiffany Wong[3]; Tiffany Wu[3]; Racquel Corpuz[3]; Bill Meilandt[3]; Ryan Kelly[3]; Felix Yeh[3]; Anne Biever[3]; Jesse Hanson[1]; John Chen[2]; John Tran[3]; [1]*Genentech, Inc., South San Francisco, CA;* [2]*NovaBioAssays, Boston, Massachusetts;* [3]*Genentech Inc, South San Francisco, CA*

DISEASE BIOMARKERS
049-063

TP 049 **A Validated LC-MS/MS Method for Quantification of 3-Bromotyrosine in Patients with EoE**; Morgan Thomas[1]; Mac Gilliland[1]; [1]*Furman University, Greenville, SC*

TP 050 **Utilization of a multi-omics integrative platform to analyze the inflamed gut tissue microenvironment**; Zohaib N. Khan[1]; Cristina C. Clement[1]; Laura Santambrogio[1]; [1]*Weill Cornell Medicine, New York, NY*

TP 051 **ProteonanoTM: a novel deep proteomics platform with picogram sensitivity and its application in Alzheimer's disease**; Dan Liu[1, 2, 3]; Feifei Hu[1, 2, 3]; Xinyan Xie[1, 2, 3]; Junyi Wang[1, 2, 3]; Yuanyuan Peng[1, 2, 3]; Yonghao Zhang[4]; Xiehua Ouyang[4]; Shanshan Lv[4]; Yanting Meng[4]; Libing Wang[4]; Ziquan Cao[4]; Yi Wang[4]; Hao Wu[4]; Yan Zeng[1, 2, 3]; [1]*Brain Science and Advanced Technology Institute, Wuhan University of Science and Technology, Wuhan, China, Wuhan, China;* [2]*Geriatric Hospital Affiliated to Wuhan University of Science and Technology, Wuhan, China;* [3]*School of Public Health, Wuhan University of Science and Technology, Wuhan, China;* [4]*Nanomics Biotechnology, Hangzhou, China*

TP 052 **Development of an effective biomarker panel for diabetic kidney disease progression by using a nanobinder assisted sample processing platform**; Ban Zhao[1, 2]; Yonghao Zhang[3]; Xiehua Ouyang[3]; Yi Wang[3]; Hao Wu[3]; Yonghui Mao[1, 2]; [1]*Department of Nephrology, Beijing Hospital, Dongcheng District, China;* [2]*National Center for Gerontology, Institute of Geriatric Medicine, Chinese Academy of Medical Sciences, Dongcheng District, China;* [3]*Nanomics Biotechnology, Hangzhou, China*

TP 053 **Identification of tumor-marker gangliosides for early cancer detection: a mass spectrometry approach**; Rachel Culp-Hill[1]; Collin Hill[1]; Adele Blackler[1]; [1]*AOA Dx, Boulder, CO*

TP 054 **Association of external exposome with metabolome in early childhood allergic diseases**; Ha Eun SONG[1]; Mi Jeong Kim[1]; Hyo Yeong Lee[1]; Su Jung Kim[1]; Hyun Ju Yoo[1]; [1]*ASAN Medical center, SEOUL, South Korea*

TP 055 **QUANTITATIVE ANALYSIS BY LC-MS/MS OF THYROID HORMONE BIOMARKERS EXTRACTED FROM BLOOD COLLECTED WITH THE TASSO MICROSAMPLING DEVICE**; Chad D. Christianson[1]; Jason S. Watts[1]; Brooke I. Whitson[1]; Jennifer S. Zimmer[1]; [1]*Alturas Analytics, Moscow, ID*

TP 056 **Evaluating Bone Marrow Lipidomic Changes and Their Potential Association with Alzheimer's Disease**; Sarah G. Clark[1]; Amie M. Solosky[1]; Charles A. Schurman[2]; Kenneth A. Wilson[2]; Lisa M. Ellerby[2]; Birgit Schilling[2]; Erin S. Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Buck Institute for Research on Aging, Novato, CA*

TP 057 **Exploring the critical role of doubly polyunsaturated phosphatidylethanolamines in the production of ferroptotic hydroperoxy lipid signals using HPLC/MS/MS**; Svetlana N. Samovich[1, 2]; Karolina Mikulska-Ruminska[3]; Haider H. Dar[2]; Yulia Y. Tyurina[2]; Vladimir A. Tyurin[2]; Austin B. Souryavong[2]; Alexander A. Kapralov[2]; Andrew A. Amoscato[2]; Ofer Beharier[4]; S. Ananth Karumanchi[5]; Claudette M. St Croix[6]; Xin Yang[7]; Theodore R. Holman[8]; Andrew P. VanDemark[9]; Yoel Sadovsky[10, 11]; Rama K. Mallampalli[12]; Sally E. Wenzel[2]; Wei Gu[7, 13]; Yuri L. Bunimovich[14]; Ivet Bahar[15]; Valerian E. Kagan[2, 16, 17, 18]; Hülya Bayır[1, 19]; *[1]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; [2]Department of Environmental and Occupational Health, Center for Free Radical and Antioxidant Health, School of Public Health, University of Pittsburgh, Pittsburgh, PA; [3]Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Torun, Poland; [4]Obstetrics and Gynecology Division, Hadassah Medical Center, Faculty of Medicine of the Hebrew University of Jerusalem, Jerusalem, Israel; [5]Department of Medicine, Cedars-Sinai Medical Center, Los Angeles, CA; [6]Department of Cell Biology, University of Pittsburgh, Pittsburgh, PA; [7]Institute for Cancer Genetics, and Herbert Irving Comprehensive Cancer Center, Vagelos College of Physicians and Surgeons, Columbia University, New York, NY; [8]Department of Chemistry and Biochemistry, University of California, Santa Cruz, CA; [9]Department of Biological Sciences, University of Pittsburgh, Pittsburgh, PA; [10]Magee-Womens Research Institute, Department of Obstetrics, Gynecology, and Reproductive Sciences, University of Pittsburgh, Pittsburgh, PA; [11]Department of Microbiology and Molecular Genetics, University of Pittsburgh, Pittsburgh, PA; [12]Department of Internal Medicine, The Ohio State University, Columbus, OH; [13]Department of Pathology and Cell Biology, Vagelos College of Physicians and Surgeons, Columbia University, New York, NY; [14]Department of Dermatology, University of Pittsburgh, Pittsburgh, PA; [15]Laufer Center for Physical and Quantitative Biology, Laufer Center, Z-5252, Stony Brook University, Stony Brook, New York; [16]Department of Radiation Oncology, University of Pittsburgh, Pittsburgh, PA; [17]Department of Chemistry, University of Pittsburgh, Pittsburgh, PA; [18]Department of Pharmacology and Chemical Biology, University of Pittsburgh, Pittsburgh, PA; [19]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 058 **Phosphoproteomics predict response to Venetoclax plus Azacitidine in Acute Myeloid Leukemia patients**; Josie A. Christopher[1]; Luis Nobre[1]; Weronika E. Borek[1]; Amy E. Campbell[1]; David N. Perkins[1]; Pedro Moreno-Cardoso[1]; Nazrath Nawaz[1]; Janet Kelsall[1]; Paolo Gallipoli[2]; Andrea Arruda[3]; Alex Ambinder[4]; Andrew Thompson[1]; Andrew Williamson[1]; Gabriel Ghiaur[4]; Sayantanee Dutta[5]; Mark D. Minden[3, 6]; David J. Britton[1]; Heinz Sill[5]; John G. Gribben[2]; Pedro R. Cutillas[1, 2]; Arran D. Dokal[1]; *[1]Kinomica Ltd, Macclesfield, Cheshire, United Kingdom; [2]Barts Cancer Institute, Queen Mary University of London, London, United Kingdom; [3]Princess Margaret Cancer Centre, University Health Network, Toronto, ON; [4]Johns Hopkins Sidney Kimmel Comprehensive Cancer Center, Baltimore, MD; [5]Division of Hematology, Medical University of Graz, Graz, Austria; [6]Department of Medical Biophysics, University of Toronto, Toronto, ON*

TP 059 **Paramagnetic Bead–Based Multi-Omics Profiling of Human Serum in Alzheimer's Disease**; Ching-Yuan Yang[1]; Haiyan Lu[2]; Michael M. Rosenblat[3]; Lingjun Li[2, 4]; *[1]Biophysics Graduate Program, University of Wisconsin-Madison, Madison, Wisconsin; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin; [3]Promega Corporation, Madison, Wisconsin; [4]Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin*

TP 060 **Unveiling Proteomic Signatures of Tau Pathogenesis through Label-Free Mass Spectrometry Analysis**; Xuemei Zeng[1]; Yijun Chen[1]; Anuradha Sehrawat[1]; Eric E. Abrahamson[1, 2]; Julia K. Kofler[1]; William R. Paljug[1, 2]; Miloslav D. Ikonomovic[1, 2]; Thomas K. Karikari[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]VA Pittsburgh Healthcare System, Pittsburgh, Pennsylvania*

TP 061 **Investigation of blood proteomic biomarkers in individuals with Nieman-Pick Disease Type C1**; Olivia C Wagner[1]; Wenping Li[1]; Derek Alexander[2]; Forbes D. Porter[2]; Stephanie M Cologna[3]; *[1]University of Illinois Chicago, Chicago, IL; [2]NIH, Bethesda, MD; [3]University of Illinois at Chicago, Chicago, IL*

TP 062 **Development of a targeted multiplexed method to measure complement activation in human ocular samples**; Yadira X Perez Paramo[1]; Erin Tom[1]; Shelby M Coates[2]; Michael C Chang[1]; Lee A Honigberg[1]; W Rodney Mathews[1]; Veronica G Anania[1]; *[1]Genentech, South San Francisco, CA; [2]Washington State University, Spokane, WA*

TP 063 **Defining the proteome, glycoproteome and lipidome by mass spectrometry in a congenital disorder of glycosylation for discovering diagnostic biomarkers**; Anu Jain[1]; Kishore Garapati[1]; Seul Kee Byeon[1]; Rohit Budhraja[1]; Wasantha Ranatunga[1]; Christina Lam[2, 3]; Matthew J. Schultz[1]; Tamas Kozicz[1, 4, 5]; Eva Morava[1, 4, 5]; Akhilesh Pandey[1]; *[1]Mayo Clinic, Rochester, MN; [2]Seattle Children's Research Institute, Seattle, United Kingdom; [3]University of Washington School of Medicine, Seattle, Washington; [4]Icahn School of Medicine at Mount Sinai, New York, NY; [5]University of Pecs Medical School, Pecs, Hungary*

ENVIRONMENTAL: GENERAL II

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TP 064 **Putative Identification of Hydroxyproline-containing Microcystins by UHPLC-MS/MS**; Sanduni H Premathilaka[1]; Judy A Westrick[2]; Dragan Isailovic[1]; *[1]University of Toledo, Toledo, OH; [2]Wayne State University, Detroit , MI*

TP 065 **Novel Separation Method of Per- and Polyfluoroalkyl Substances Via 2D LC×DMS-MS2**; Christopher Ryan[1]; Emir Nazdrajić[1]; J. Larry Campbell[2]; W. Scott Hopkins[1, 3, 4]; *[1]University of Waterloo, Waterloo, ON; [2]Bedrock Scientific Inc, Milton, ON; [3]Watermine Innovation, Waterloo, ON; [4]Centre for Eye and Vision Research, Hong Kong, Hong Kong*

TP 066 **Analytical Characterization of Cannabis Flower Buds by LC-MS and ICP-MS**; Kingsley K Donkor[1]; Nicole Hanna[1]; Devansh Sharma[1]; Tharusha Jayasinghe[1]; *[1]Thompson Rivers University, Kamloops, BC*

TP 067 **Investigation of Thermal Decomposition Poly-Fluoroalkyl Substances (PFAS) with Thermal Desorption – Pyrolysis – Gas Chromatography-Mass Spectrometry**; Katerina Litvanova[1]; Bethany Klemetsrud[2]; Feng Xiao[3]; Alena Kubatova[1]; *[1]University of North Dakota, Grand Forks, ND; [2]Department of Chemical Engineering, University of North Dakota, Grand Forks, ND; [3]University of Missouri-Columbia, Columbia, MO*

TP 068 **Quantification of Brominated Flame Retardants in Polymer Samples Using Direct Mass Spectrometric Analysis**; Krista Grönlund[1]; Ville Nissinen[1]; Kirsi Korpijärvi[2]; Milad Mosallaei[3]; Ilkka Rytöluoto[3]; Jani Pelto[3]; Mika Suvanto[1]; Jarkko J. Saarinen[1]; Janne Jänis[1]; *[1]University of Eastern Finland, JOENSUU, Finland; [2]VTT Technical Research Centre of Finland Ltd., Jyväskylä, Finland; [3]VTT Technical Research Centre of Finland Ltd., Tampere, Finland*

TP 069 **Automated targeted and non-targeted LC-Orbitrap MS workflow for analysis of more than 40,000 PFAS compounds**; Cynthia M Grim[1]; Toby Astill[1]; Valérie Thibert[2]; Aristide Ganci[2]; Bénédicte Gauriat[2]; Richard Cochran[3]; P Lee Ferguson[4]; Jean-François Garnier[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Courtaboeuf, France; [3]Thermo Fisher Scientific, Bannockburn, IL; [4]Department of Civil and Environmental Engineering and Nicholas School of the Environment, Duke University, Durham, NC*

TP 070 **Real Time Monitoring of Semi-Volatile Emerging Atmospheric Contaminants: Application of the AIM Reactor in PFAS Detection**; Omar El Hajj[1]; Spiro Jorga[2]; Abigail Koss[1]; Veronika Pospisilova[2]; Wade Bontempo[1]; Joel Kimmel[1]; *[1]Tofwerk USA, Boulder, CO; [2]TOFWERK AG, Thun, Switzerland*

TP 071 **Cyanobacterial classification using a DART-Orbitrap mass spectrometer**; Yuya Takai[1]; Wakana Hosoe[2]; Yuka Tsuboi[2]; Shunichi Ishikawa[2]; Hana Kozaki[2]; Masaki Hoshino[2]; Masahiko Tachi[3]; Hajime Mizuno[2]; Susumu Y. Imanishi[2]; *[1]Meijo University, Nagoya, Japan; [2]Meijo University, Nagoya, Japan; [3]Aichi Prefectural Institute of Public Health, Nagoya, Japan*

TP 072 **Association between plasma metabolites and heavy metal exposure in residents of environmentally polluted areas**; Mi Jeong Kim[1]; Ha Eun SONG[1]; Hyo Yeong Lee[1]; Su Jung Kim[1]; Hyun Ju Yoo[1]; *[1]ASAN Medical center, SEOUL, South Korea*

TP 073 **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[1]; Patrick T Justen[1]; Amy A Cuthbertson[1]; Ashley A Perkins[1]; Vincent Esposito[1]; Hannah K Liberatore[1]; Susan D Richardson[1]; *[1]University of South Carolina, Columbia, SC*

TP 074 **Analysis of PFAS and other environmental contaminants in soil and oat plants using high resolution GC/MS**; Sofia Nieto[1]; Matthew Giardina[1]; Matthew Curtis[1]; Luann Wong[2]; Gabrielle Black[2]; Thomas Young[2]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]University of California, Davis, Davis, CA*

TP 075 **Studies of the adsorption process of organic pollutants on microplastics using high-throughput SPME-MOI-LEI-MS**; Tommaso Grazioso[1]; Adriana Arigò[1]; Giorgio Famiglini[1]; Pierangela Palma[1, 2]; ACHILLE CAPPIELLO[1, 2]; *[1]Università degli studi di Urbino Carbo Bo, Urbino, Italy; [2]Vancouver Island University, Nanaimo, BC*

TP 076 **Faster Analysis for Forever Chemicals: Accelerating PFAS Analysis with UPLC-HRIM-MS**; Alan McKenzie-Coe[1]; Thomas Lubinsky[1]; Jeremy P. Koelmel[2]; Emma E. Rennie[3]; David A Weil[3]; Sarah M. Stow[3]; Paul Stelben[2]; Krystal J. Godri Pollitt[4]; David Godri[5]; Frederick Strathmann[1]; Daniel DeBord[6]; *[1]MOBILion Systems, Chadds Ford, PA; [2]Innovative Omics, Sarasota, FL; [3]Agilent Technologies, Santa Clara, CA; [4]Yale University, New Haven, CT; [5]3rd Floor Solutions, Toronto, Ontario; [6]MOBILionSystems, Chadds Ford, PA*

TP 077 **Systematic Study of Techniques to Minimize PFAS Background Interferences**; Om K Shrestha[1]; Kathleen K Luo[1]; Megan Davis[1]; Landon A Wiest[1]; Evelyn H Wang[1]; Xiaomeng Xia[1]; Keith Herman[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

TP 078 **Complementary Quantitative and Qualitative Mass Spectrometry Analysis for Environmental Samples**; Kendra Selby[1]; Stephanie Shan[1]; Summy Shrestha[1]; Claire Korte[1]; M Nazim Boutaghou[2]; Samantha A Olendorff[2]; Kevin R Tucker[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL; [2]Shimadzu Scientific Instruments, Columbia, MD*

TP 079 **Physicochemical Properties and Partitioning Behaviour of para-Phenylenediamine quinones (PPDQs) Investigated with Direct Mass Spectrometry**; Misha Zvekic[1, 2]; Joseph Monaghan[1, 2]; Angelina Jaeger[1, 2]; Chris G Gill[1, 2, 3, 4]; Erik T Krogh[1, 2]; *[1]Vancouver Island University, Nanaimo, BC; [2]University of Victoria, Victoria, BC; [3]Simon Fraser University, Burnaby, BC; [4]University of Washingon, Seattle, WA*

TP 080 **Extraction Optimization and Non-Targeted Analyses of Per- and Polyfluoroalkyl Substances (PFAS) in Mammalian Milk**; Kara M Joseph[1]; Gregory Kudzin[1]; Anna K. Boatman[1]; Erin S. Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

TP 081 **Classification and identification of cyanobacteria in frozen samples using MALDI Biotyper**; Sakura Kawasaki[1]; Haruka Okuma[1]; Takahiro Wakayama[1]; Kosuke Hatanaka[1]; Yuka Maruoka[1]; Hajime Mizuno[1]; Susumu Y. Imanishi[1]; *[1]Meijo University, Nagoya, Japan*

TP 082 **Photoionization High-Resolution Mass Spectrometry for Analysis of Atmospheric Particulate Matter**; Hendryk Czech[1, 2]; Patrick Martens[1]; Sven Ehlert[3]; Paul Kösling[1]; Marco Schmidt[1]; Christopher Rüger[1]; Johannes Passig[1, 2]; Thorsten Streibel[1, 2]; Martin Rigler[4]; Andreas Walte[3]; Ralf Zimmermann[1, 2]; *[1]University of Rostock, Rostock, Germany; [2]Joint Mass Spectrometry Centre, Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Munich, Munich, Germany; [3]Photonion GmbH, Schwerin, Germany; [4]Aerosol Magee Inc., Ljubljana, Slovenia*

TP 083 **New approach for assigning emerging contaminants from high-resolution mass spectrometry data – comprehensive screening and Kendrick mass defect network analysis**; Laura Tenhumberg[1]; Alessandro Vetere[2]; Wolfgang Schrader[2]; *[1]Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany; [2]Max-Planck-Institut für Kohlenforschung, 45470 Mülheim an der Ruhr, Germany*

TP 084 **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[1]; Tae-Young Kim[1]; *[1]School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea*

TP 085 **Unveiling the hidden threat: Paint microplastics and their extractable organics in soil**; Woo-Young Song[1]; Shin Woong Kim[2, 3]; Walter R. Waldman[4]; Matthias C. Rillig[2, 3]; Tae-Young Kim[1]; *[1]School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea; [2]Institute of Biology, Freie Universität Berlin, Berlin, Germany; [3]Berlin-Brandenburg Institute of Advanced Biodiversity Research, Berlin, Germany; [4]Science and Technology Center for Sustainability, Federal University of São Carlos, São Carlos, Brazil*

TP 086 **Detecting PFAS beyond the Current Regulative Request: a Comprehensive Overview of the Contamination in Water by UPHLC-Ion mobility-HRMS**; Arnd Ingendoh[1]; Igor Nikitin[1]; Carsten Baessmann[1]; Andrea Kiehne[1]; Eva-Maria Niehaus[1]; *[1]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany*

TP 087 **Evaluation of DESI mounted on Q-Tof and TQ mass spectrometers to image PFAS compounds in different matrices**; Emmanuelle Claude[1]; Alexandra Lee[1]; Mujeebatu Kadiri-Asamoah[1]; Stuart Adams[1]; Emrys Jones[1]; Joanne Ballantyne[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

TP 088 **Untargeted Screening for PFAS Chemicals Using Comprehensive Feature Detection**; Jeff Goshawk[1]; Andrew Tudor[1]; Sarah Dowd[2]; Jonathan Fox[1]; Hania Khoury-Hollins[1]; Michael McCullagh[1]; Isabel Riba[1]; Susan Slade[1]; Russell Mortishire-Smith[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, Massachusetts*

TP 089 **Identification of short chain per and polyfluorinated alkyl substances (PFAS) using ion ratios with low mass product ions**; Kieron Faherty[1]; Stuart J Adams[2]; Kate Whyatt[2]; David Gordon[2]; *[1]Waters Corporation, Milford,* *Massachusetts; [2]Waters Corporation, Wilmslow, United Kingdom*

TP 090 **A novel approach to identifying Environmental Risk Factors for Breast Cancer Through Integrated Untargeted and Targeted HSA Adductomics**; Fariba Tayyari[1]; Aishwarya Jala[1]; Yeunook Bae[1]; Cathelin Huang[1]; James Burke[1]; Kwang-Youn Kim[1]; Kalliopi Siziopikou[1]; Alexander White[2]; Dale Sandler[2]; William E Funk[1]; *[1]Northwestern University, Chicago, IL; [2]NIH/NIEHS, Research Triangle Park, NC*

TP 091 **Expanding the known chemical universe for vehicle tire related emerging contaminants with complementary non-targeted analysis (NTA) approaches**; Mauricius Marques Dos Santos[1]; Isaac Wai Loon Law[1]; Shane Allen Snyder[1]; *[1]Nanyang Technological University (NTU)- NEWRI, Singapore, Singapore*

TP 092 **Analysis of PFAS in Potable Water by Direct Injection Using the LCMS-8060NX**; Luis O Junqueira[1]; Marcos A Pudenzi[1]; Lucas L Zanin[1]; Ichiro Hirano[1]; *[1]Shimadzu do Brasil, Barueri, Brazil*

TP 093 **Characterization of PFAS chemicals in anti-fog solutions using gas chromatography and high-performance time-of-flight mass spectrometry**; Katie Redinius[1]; David E Alonso[2]; Joe Binkley[1]; *[1]LECO Corporation, Saint Joseph, MI; [2]Leco Corporation, St. Joseph, MI*

TP 094 **Analysis of PFAS in water using Head-Space Solid Phase Microextraction-Gas Chromatography/Mass Spectrometry (HS-SPME GCMS)**; Andy Sandy[1]; Evelyn Wang[1]; Yoshiyuki Okamura[1]; Ruth Marfil-Vega[1]; Alan Owens[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

TP 095 **Expanding Molecular Compositional Coverage of Water-Soluble Emerging Contaminants with Liquid Chromatography – Ultrahigh-Resolution Mass Spectrometry**; Joseph W. Frye-Jones[1, 2]; Martha L. Chacon-Patino[1, 3]; Lissa C. Anderson[1]; Alvaro J. Tello-Rodriguez[1, 4]; Winston K. Robbins[1]; Alan G. Marshall[1, 2]; Ryan P. Rodgers[1, 2, 3, 5]; *[1]National High Magnetic Field Laboratory, Tallahassee, Florida; [2]Florida State University - Department of Chemistry and Biochemistry, Tallahassee, FL; [3]International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France; [4]Florida State University, Tallahassee, FL; [5]Université de Pau et des Pays de l'Adour, Pau, France*

TP 096 **Simultaneous Identification and Quantification of Lignin Breakdown Products by Thermal Desorption Pyrolysis Gas Chromatography Mass Spectrometry Methanizer Flame Ionization Detector**; Mason L Clobes[1]; Md Musfiqur Rahman[1, 2]; Nafisa Bala[1]; Alena Kubatova[1]; *[1]University of North Dakota, Grand Forks, ND; [2]Winder Laboratories, Winder, GA*

TP 097 **Peekaboo, PFAS in fabrics and textiles, we see you**; Zijie Xia[1]; Sawyer Schugel[1]; Pheng Yang[1]; Brian Beall[1]; *[1]Claros Technologies, Minneapolis, MN*

TP 098 **Optimizing Orbitrap-based isotopic analysis of nitrate by coupling Orbitrap-MS with chromatographic separation techniques**; Allyson Girard[1]; Justin Y Elliott[1]; J. David Felix[1]; Hussain Abdulla[1]; *[1]Texas A&M University-Corpus Christi, Corpus Christi, TX*

TP 099 **Investigating electron shuttling within the dissolved organic matter pool of an Iron-oxidizing microbial community using high-resolution Tandem Mass Spectrometry**; Tilman Schramm[1]; Cristina Escudero Parada[2]; Paolo Stincone[2]; Abzer Shah[2]; Franziska Schädler[2]; Lars Grimm[2]; Marie Mollenkopf[2]; Verena Nikeleit[2]; Andreas Kappler[2]; Daniel Petras[1]; *[1]University of California, Riverside, Riverside, CA; [2]University of Tuebingen, Germany, Tuebingen, Germany*

EXPOSOMICS
100-118

TP 100 **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[1]; Yuliet Monatukwa[1]; Allysha O'Donnell[1]; Abdur Rahim[1]; Andrew Rajczewski[1]; Joshua Gann[1, 2]; Alexander Hurben[1, 3]; Gunnar Boysen[4]; Natalia Tretyakova[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Vanderbilt University, Nashville, TN; [3]University of California, Berkeley, Berkeley, CA; [4]University of Arkansas for Medical Sciences, Little Rock, AR*

TP 101 **The chemical exposome in glioblastoma and its potential connection with ultrafine particles**; Ruben Gil-Solsona[1, 2]; Daniel Gutierrez-Martin[1]; Albert Pons-Escoda[3, 4]; Carles Majos[3, 4]; Noemi Vidal[4, 5]; Fulvio Amato[1]; Maria Christina Nika[1]; Pablo Gago Ferrero[6]; *[1]IDAEA-CSIC, Barcelona, Spain; [2]National and Kapodistrian University of Athens Medical School, Athens, Greece; [3]Radiology Department, Hospital Universitari de Bellvitge, Barcelona, Spain; [4]Neuro-Oncology Unit, Institut d'Investigació Biomedica de Bellvitge, IDIBELL, Barcelona, Spain; [5]Deparment of Pathology, Hospital de Bellvitge, Barcelona, Spain; [6]Institute of Environmental Assessment and Water Research - Spanish Council for Scientific Research (IDAEA-CSIC), Barcelona, Spain*

TP 102 **An Assessment of Serum Lipidomic Perturbations due to Drinking Water and Occupational PFAS Exposures**; Ashlee T Falls[1]; Anna K. Boatman[2]; Kaylie I Kirkwood-Donelson[3]; Heather M. Stapleton[4]; Erin S. Baker[2]; *[1]University of North Carolina - Chapel Hill, Chapel Hill, NC; [2]University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]National Institute of Environmental Health Sciences, Durham, NC; [4]Duke University, Durham, NC*

TP 103 **A Multidimensional Database for the Detection of Quaternary Ammonium Compounds and Their Phase I Metabolites in Humans**; Ryan Nguyen[1]; Ryan P. Seguin[1]; Dylan H. Ross[2]; Pengyu Chen[1]; Sean H. Richardson[3]; Jennifer Liem[4]; Yvonne S. Lin[4]; Libin Xu[1]; *[1]Department of Medicinal Chemistry, University of Washington, Seattle, WA; [2]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [3]Department of Mathematics, University of Washington, Seattle, WA; [4]Department of Pharmaceutics, University of Washington, Seattle, WA*

TP 104 **Evaluating Environmental Factors in Systemic Autoimmune Rheumatic Diseases with Non-Targeted Analyses of Patients and Their Unaffected Siblings**; Gregory Kudzin[1]; James N. Dodds[1]; Kaylie I. Kirkwood-Donelson[2]; Adam Schiffenbauer[3]; Frederick W. Miller[3]; Kakali Sarkar[3]; Payam Noroozi Farhadi[3]; Alan K. Jarmusch[4]; Lisa G. Rider[3]; Erin S. Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]National Institute of Environmental Health Sciences, Durham, NC; [3]Environmental Autoimmunity Group, Clinical Research Branch, National Institute of Environmental Health Sciences, Bethesda, MD; [4]Immunity, Inflammation, and Disease Laboratory, National Institute of Environmental Health Sciences, Durham, NC*

TP 105 **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[1]; Jody C May[1]; Katrina L Leaptrot[1]; Alexandra C Rutledge-Schrimpe[1]; Simona G Codreanu[1]; Jerry D Holman[1]; Hania Khoury-Hollins[2]; Lee A Gethings[2]; Stacy D Sherrod[1]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]Waters Corporation, Wilmslow, United Kingdom*

TP 106 **Characterization of reactive electrophiles-derived exposome by profiling urinary mercapturic acid conjugates using enzymatic deacetylation and data-independent acquisition mass spectrometry**; Yuan-Chih Chen[1]; Pao-Chi Liao[1]; *[1]National Cheng Kung University, Tainan, Taiwan*

TP 107 **Discovery of Noninvasive Biomarkers for Radiation Exposure via LC-MS-based Hair Metabolomics**; Huan Zhang[1, 2]; Rui Xui[1, 2]; Shruthi Kandalai[1, 3, 4]; Haidong Peng[1, 3, 4]; Michael Geiman[1, 3]; Shuaixin Gao[1, 2]; Naduparambil K. Jacob[1, 3]; Qingfei Zheng[1, 3, 4]; Jiangjiang Zhu[1, 2]; *[1]Comprehensive Cancer Center, The Ohio State University, Columbus, OH, 43210; [2]Human Nutrition Program,* *Department of Human Sciences, The Ohio State University, Columbus, OH, 43210; [3]Department of Radiation Oncology, College of Medicine, The Ohio State University, Columbus, OH, 43210; [4]Center for Cancer Metabolism, The Ohio State University, Columbus, OH, 43210*

TP 108 **A mass spectrometry-based scalable workflow for exposome research**; Xiangping Lin[1]; Xinyue Zhang[1]; Michael P. Snyder[1]; *[1]Department of Genetics, Stanford University School of Medicine, Stanford, CA*

TP 109 **Label-free protein expression analysis from mammalian tissues following dermal exposure to perfluorobutanoic acid**; Madison P. Cooper[1]; Stacey E. Anderson[1]; Lisa M. Weatherly[1]; Laurel G. Jackson[1]; Ewa Lukomska[1]; Justin M. Hettick[1]; *[1]NIOSH, Morgantown, WV*

TP 110 **Assessment of exposure to oxybenzone, synthetic antioxidants and triclosan using targeted and untargeted LC-MS/MS of urine samples**; Said Matar[1, 2]; Lekha Sleno[1, 2]; *[1]University of Quebec in Montreal, Montreal, QC; [2]EcotoQ research network on ecotoxicology research, Montreal, QC*

TP 111 **Hair as a high-value matrix for exposomics: multi-residue analysis of xenobiotics by LC-HRMS**; Delia Castilla-Fernández[1]; Benedikt Warth[1]; *[1]University of Vienna, Department of Food Chemistry and Toxicology, Faculty of Chemistry, Vienna, Austria., Vienna, Austria*

TP 112 **Enhanced Coverage of volatile and semi-volatile PFAS Using Experimental and Predicted GC-HRMS PCI and EI libraries**; Jeremy Koelmel[1]; Elizabeth Z. Lin[1]; Emily Johnson[1]; Paul Stelben[1]; Sheng Liu[1]; Kozo Nishida[2]; Hiroshi Tsugawa[2]; Ashley Lin[3, 4]; Yakun Zhou[1]; Vladimir Nikiforov[5]; Alexander Aksenov[6]; Joseph Okeme[1]; John Bowden[7]; Krystal Godri Pollitt[1]; *[1]Yale University, New Haven, CT; [2]Tokyo University of Agriculture and Technology, Koganei-shi, Japan; [3]University of Florida, Gainesville, FL; [4]University of Florida, GAINESVILLE, FL; [5]NILU, Kjeller, Norway; [6]University of Connecticut, Storrs, CT; [7]University of Florida Department of Chemistry, Gainesville, FL*

TP 113 **Urine metabolomics analysis of dermal exposure to spray polyurethane foam**; Chani Sahabandu Hewa Sahabanduge[1]; Kushal Biswas[1]; Dhimiter Bello[1]; Pengyuan Liu[2]; *[1]University of Massachusetts Lowell, Lowell, MA; [2]University of Massachusetts, Lowell, Lowell, MA*

TP 114 **Leveraging the MS1 Dimension and Formula Prediction in Non-Targeted Analysis of PFAS using New FluoroMatch Algorithms: Assessing Confidence and Coverage**; David Schiessel[1]; Jeremy Koelmel[2]; Michael Kummer[1]; David Godri[3]; Sheng Liu[2]; Elizabeth Z. Lin[2]; John Bowden[4]; Olivier Chevallier[5]; Camden G. Camacho[4]; Emma Rennie[2]; Krystal Godri Pollitt[2]; *[1]Innovative Omics, Sarasota, FL; [2]Yale University, New Haven, CT; [3]3rd Floor Solutions, Toronto, Ontario; [4]University of Florida, Gainesville, FL; [5]Agilent Technologies, Santa Clara, CA*

TP 115 **MRM-profiling for detecting emerging contaminants in human biomonitoring: Application to Bisphenol A replacements**; Jasmin Chovatiya[1]; Ravikumar Jagani[1]; Manish Arora[1]; Syam S. Andra[1]; *[1]Institute for Exposomic Research, Department of Environmental Medicine and Public Health, New York, NY*

TP 116 **Evaluating Lipidomic Changes in Mice Exposed to Wildfire-Relevant Smoke from Different Fuel and Burn Conditions**; Haley C. Jostes[1]; Amie M. Solosky[1]; Jessie R. Chappel[2]; Celeste Carberry[1]; Julia E. Rager[1]; Erin S. Baker[1]; *[1]UNC-Chapel Hill, Chapel Hill, NC; [2]North Carolina State University, Raleigh, NC*

TP 117 **A Lipidomic Exploration of the Impact of Perfluorooctanoic Acid (PFOA) Exposure on SARS-CoV-2 Infection**; Allison N. Fry[1]; Jessie R. Chapel[2]; Amie M. Solosky[1]; Kara M. Joseph[1]; Sarah G. Clark[1]; Deanna Lanier[3]; Mario Uchimiya[3]; Dawne Rowe[4]; David A. Gaul[5]; Facundo M. Fernandez[5]; S. Mark Tompkins[4]; Tracey Woodlief[6]; Jamie DeWitt[7]; Arthur Edison[3]; Erin S. Baker[1]; *[1]Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Bioinformatics Research Center, Department of Biological Sciences, North Carolina State University, Raleigh, NC; [3]Complex Carbohydrate Research Center, University of Georgia, Athens, GA; [4]Center for Vaccines and Immunology, University of Georgia, Athens, GA; [5]School of Chemistry and Biochemistry, Georgia Institute of Technology, Altanta, GA; [6]Department of Pharmacology and Toxicology, Brody School of Medicine, East Carolina University, Greenville, NC; [7]Department of Environmental and Molecular Toxicology, Oregon State University, Corvallis, OR*

TP 118 **Exploring Proteomic Signatures Linked to Early Life Exposome in Atopic Dermatitis and Asthma : ECHO-COCOA Study**; Seungyoon Seo[1]; Yeonwoo Jo[1]; Hwangkyo Jeong[1]; Hosub Im[2]; Mi-Jin Kang[3]; Soo-Jong Hong[4]; Jeonghun Yeom[1]; *[1]Prometabio Research Institute, prometabio co., ltd., Hanam-si, South Korea; [2]Institute for Life & Environmental Technology, Smartive Corporation, Hanam-si, South Korea; [3]Humidifier Disinfectant Health Center, Asan Medical Center, Songpa-gu, South Korea; [4]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

119-139

TP 119 **Determination of Limonin in Citrus Flour by Time of Flight (TOF) LC/MS**; Sue D'Antonio[1]; Donna Payne[2]; John Wright[3]; Michael Adams[4]; *[1]Agilent Technologies Inc., Cedar Creek, TX; [2]AnalytEval, SMITHVILLE, TX; [3]Agilent Technologies, Wilmington, DE; [4]CWC Labs, Cedar Creek, TX*

TP 120 **Overcoming Sampling Challenges in Analyzing Retained Tea Flavor Using Soft Ionization by Chemical Reaction in Transfer (SICRIT)**; Xinwei Feng[1]; Hui Li[1]; Ying Xu[1]; *[1]The Coca-Cola Company, Shanghai, China*

TP 121 **Metabolic Remodeling During Fructification of Enoki Mushroom**; Chikondi Shaba[1]; Pawel L. Urban[1]; *[1]National Tsing Hua University, Hsinchu City, Taiwan*

TP 122 **Continued Method Development of a Quantitative Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) Method for Analyzing Diarrhetic Shellfish Toxins**; Christopher R. Beekman[1]; Brigid Carr[2]; Daniel Chavez[3]; Shelley K. Lankford[3]; Stephen D. Archer[2]; Jonathan R. Deeds[1]; *[1]U.S. Food and Drug Administration, College Park, MD; [2]Bigelow Laboratory for Ocean Sciences, East Boothbay, ME; [3]Washington State Department of Health Public Health Laboratories, Shoreline, WA*

TP 123 **Proteomics for species authentication of cod and corresponding fishery products**; Han-ju Chien[1]; Yu-Han Huang[2]; Yi-Feng Zheng[3]; Wei-Chen Wang[3]; Cheng-Yu Kuo[3]; Guor-Jien Wei[2, 4]; Chien-Chen Lai[3, 5, 6]; *[1]Department of Biochemical Science and Technology, National Chiayi University, Chiayi city, Taiwan; [2]Institute of Food Safety and Health Risk Assessment, National Yang-Ming University, Taipei city, Taiwan; [3]Institute of Molecular Biology, National Chung Hsing University, Taichung city, Taiwan; [4]Metabolomics-Proteomics Research Center, National Yang-Ming University, Taipei city, Taiwan; [5]Advanced Plant Biotechnology Center, National Chung Hsing University, Taichung city, Taiwan; [6]Graduate Institute of Chinese Medical Science, China Medical University, Taichung city, Taiwan*

TP 124 **Multiomic Analysis for Identifying Adulteration, Geographical Origins, and Species in Soy Sauce**; Wei-chen Wang[1]; Shau-Chun Wang[2]; Chien-Chen Lai[3, 4, 5, 6]; *[1]National Chung Hsing University, Taichung, Taiwan; [2]National Chung Cheng University, Chiayi city, Taiwan; [3]Institute of Molecular Biology, National Chung Hsing University, Taichung, Taiwan; [4]Advanced Plant Biotechnology Center, National Chung Hsing University, Taichung city, Taiwan; [5]Ph.D. Program in Translational Medicine, National Chung Hsing University, Taichung,* *Taiwan; [6]Rong Hsing Research Center for Translational Medicine, National Chung Hsing University, Taichung, Taiwan*

TP 125 **Analyzing Nitrosamines with Hydrogen Carrier Gas: GC/MS/MS Analysis of Nitrosamines in Sartan Drugs**; Soma Dasgupta[1]; Parul Angrish[2]; Anastasia Andrianova[3]; Joel Ferrer[2]; *[1]Agilent technologies, Bangalore, India; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent Technologies, Wilmington, DE*

TP 126 **Development of a generic fish MS detection method for allergen control**; Justin Marsh[1]; Tengfei Li[1]; Joseph Baumert1[1]; Philip Johnson[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

TP 127 **Identification of covalent protein-flavonoid interactions using intact and bottom-up mass spectrometry**; P. Matthew Joyner[1]; Abigail Martinez Valdovinos[1]; Alyssa Hornback[1]; *[1]Pepperdine University, Malibu, CA*

TP 128 **Novel Analytical Approach to The Quantitation of Bovine Immunoglobulin G Using Isoform-Specific Peptide Markers and Liquid Chromatography – Mass Spectrometry**; Stefan Ehling[1]; Matthew K Fleshman[1]; *[1]Abbott Nutrition, Columbus, OH*

TP 129 **Exploring the Impact of Protein Digestibility on Food Allergenicity through DIA-MS Profiling**; Chee Fan TAN[1]; Ai Che YAP[2]; Felicia Yu Yin ONG[1]; Hui Ru TAN[3]; Yao Xing WONG[3]; Weibiao ZHOU[2]; Juan DU[3]; Xuezhi Bi[1, 3]; *[1]Bioprocessing Technology Institute, Agency for Science, Technology and Research, Singapore, Singapore; [2]Department of Food Science and Technology, National University of Singapore, Singapore, Singapore; [3]Food, Chemical and Biotechnology Cluster, Singapore Institute of Technology, Singapore, Singapore*

TP 130 **Calibrant extraction and digestion for the development of an MS gluten detection method in fermented and hydrolyzed foods**; Sara K Schlange[1]; Joseph L Baumert[1]; Melanie L Downs[1]; *[1]University of Nebraska-Lincoln, Lincoln, NE*

TP 131 **Combining Proteomics and Metabolomics to Assess Food Protein Digestibility**; Cheng-Yu Weng[1]; Shawn Ehlers-Cheang[1]; Nikita Bacalzo[1]; Emelie Strandberg[2]; Fangzhou Li[3]; Mariana Barboza[4]; Justin B. Siegel[1]; Ilias Tagkopoulos[3]; Keith Baar[2]; Carlito B. Lebrilla[1]; *[1]Department of Chemistry, University of California, Davis, Davis, CA; [2]College of Biological Sciences, University of California, Davis, Davis, CA; [3]Department of Computer Science, University of California, Davis, Davis, CA; [4]Innovation Institute for Food and Health, University of California, Davis, Davis, CA*

TP 132 **Discrimination of foodborne pathogens associated with outbreaks using Tandem Liquid Chromatography Ion Mobility Mass Spectrometry (LC-IM-MS/MS)**; Jessica S. Pizzo[1]; Sheba P. Maaji[1]; Iffat Jerin[1]; Kimberly Y. Kartowikromo[1]; Orobola E. Olajide[1]; Ahmed M. Hamid[1]; *[1]Auburn University, AUBURN, AL*

TP 133 **Non-targeted metabolomics analysis for structural elucidation of tannins using high-resolution mass spectrometry**; HONG-JHANG CHEN[1]; GUI-RU XIE[1]; *[1]Institute of Food Science and Technology, National Taiwan University, Taipei, Taiwan*

TP 134 **Prevention of age-related diseases by taking Black chokeberry**; Takuya Yamane[1, 2]; Yu Nakajima[1]; Momoko Imai[1, 2]; Takeshi Bamba[2, 3]; Susumu Uchiyama[1, 2]; *[1]Osaka University, Suita, Japan; [2]BYU-Analytica Inc., Osaka, Japan; [3]Kyushu university, Fukuoka, Japan*

TP 135 **Chemical profiling and quantification of major royal jelly protein of royal jelly products using non-targeted and targeted metabolomics**; HONG-JHANG CHEN[1]; CHUN-CHIEH CHANG[2]; GUI-RU XIE[1]; *[1]Institute of Food Science and Technology, National Taiwan University, Taipei, Taiwan; [2]Hsinlin Biomedical Co., Ltd., Yilan, Taiwan*

TP 136 **Analysis of Pharmacokinetics of Whole Coffee Fruit Caffeine Extract in Human Serum by Liquid Chromatography Mass Spectrometry**; Nebiyu Abshiru[1]; Zb Pietrzkowski[2]; Boris Nemzer[2, 3]; *[1]FutureCeuticals, Momence, IL; [2]VDF FutureCeuticals, Inc., Momence, IL; [3]University of Illinois at Urbana-Champaign, Urbana, IL*

TP 137 **The Elemental Palette: Ionomic profiling across 500 diverse food samples**; Jacqueline Michelle Chaparro[1]; Rachel R Jones[1]; John C Evans[1]; Macy Gruszczynski[1]; Margaret Read[1]; Susan B Mitchell[1]; Melanie T Odenkirk[1]; Corey D Broeckling[1]; Tracy Shafizadeh[2]; Steven Watkins[2]; Jessica E Prenni[1]; *[1]Colorado State University, Fort Collins, CO; [2]Verso Biosciences, Davis, CA*

TP 138 **Determination of87 veterinary drug, pesticide and mycotoxin residues in beef by ionic liquid-dispersive liquid-liquid microextraction/liquid chromatography-mass spectrometry**; Sandy SO Mookantsa[1, 2]; Simiso Dube[1]; Mathew MM Nindi[1]; *[1]University of South Africa, , Florida Park, Roodepoort, South Africa; [2]Botswana National Veterinary Laboratory, Gaborone, Botswana*

TP 139 **Comparison of protein changes in donor human milk after Holder pasteurization, high-pressure process and UV-C treatment**; Bum Jin Kim[1]; Hussein M.H. Mohamed[1]; Austin Lowder[2]; Joy Waite-Cusic[1]; David Dallas[1]; *[1]Oregon State University, Corvallis, OR; [2]JBT Corporation, Erlanger, KY*

FUNDAMENTALS: ION MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS

140-156

TP 140 **The Energy Dependence of Transuranic Cation Reactions with Methane Observed by ICP-MS/MS**; Richard Cox[1]; Amanda D. French[1]; Kali M. Melby[1]; Michael J. Rodriguez[1]; Wenjin Cao[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TP 141 **Comparison of solution and gas phase structural ensembles of denatured cytochrome c**; Rebecca L Cain[1]; Ian K Webb[1]; *[1]Indiana University Purdue University Indianapolis, Indianapolis, IN*

TP 142 **Complexation of Phosphate Groups with Diserinol Isophthalamide in Electrospray Ionization Mass Spectrometry**; Neil A Ellis[1]; Madeline Schultz[1]; Daniel A Thomas[1]; *[1]University of Rhode Island, Kingston, RI*

TP 143 **Developing various length gaseous electrostatic to covalent crosslinkers: towards understanding the effects of solvation and desolvation on protein structure**; Kacy L Black[1]; Ian K. Webb[1]; *[1]IUPUI, Indianapolis, IN*

TP 144 **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[1]; Hilkka I Kenttämaa[1]; Keriany Fuentes[2]; Charles M Pletcher[1]; Jack C Howard[1]; Daria T Tsoneva[1]; *[1]Purdue University, West Lafayette, IN; [2]University of Puerto Rico Humacao, Humacao, Puerto Rico*

TP 145 **Probing Metal Ion Adduction in the Charged Residue Mechanism of ESI via Gas-Phase Ion-ion Chemistry**; Alexander M. Koers[1]; Nicole M. Brundridge[1]; Scott A. McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

TP 146 **Protecting ETD Singly-charged Products from Further Reaction via Enhanced Singly-charged Scans**; Seth A. Horn[1]; Kimberly C. Fabijanczuk[1]; Ian J. Carrick[1]; Scott A. McLuckey[1]; *[1]Purdue University Department of Chemistry, West Lafayette, IN*

TP 147 **Nitrosation of the One-Electron Oxidized Guanine and 9-Methylguanine by Nitric Oxide**; Jonathan Benny[1, 2]; Jianbo Liu[1, 2]; *[1]The Graduate Center of the City University of New York, New York, NY; [2]Queens College CUNY, Flushing, NY*

TP 148 **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[1, 2]; Jonathan Benny[1, 2]; Jianbo Liu[1, 2]; *[1]Queens College CUNY, Flushing, NY; [2]The Graduate Center of the City University of New York, New York, NY*

TP 149 **Ion Parking in a Home-Built Digital 3D Quadrupole Ion Trap: Expected Challenges and Relevant Calculations**;

Liangxuan Fu[1]; Scott A. McLuckey[1]; *[1]Purdue University Department of Chemistry, West Lafayette, IN*

TP 150 **Understanding ligand-exchange of Ni and Fe complexes on surfaces using ion soft-landing**; Raquel Cericatto Konzen[1]; Hugo Y. Samayoa-Oviedo[1]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN*

TP 151 **Origin of the unexpected Rb+ (or K+) detection from collisional activation of sodiated cyclodepsipeptides**; Chenqin Cao[1]; Sophie Liuu[2]; Ekaterina Darii[3]; Yves Gimbert[4]; Annelaure DAMONT[1]; Olivier Firmesse[2]; François FENAILLE[1]; Jean-Claude Tabet[1, 4]; *[1]Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), MetaboHUB, Gif-sur-Yvette, France; [2]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; [3]Génomique métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry, France., Evry, France; [4]Faculté des Sciences et de l'Ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Sorbonne Université, Paris, France*

TP 152 **Top-down characterization of intact proteins via on-line charge-stripping and electron capture dissociation**; Yury V. Vasilev[1]; Michael C. Hare[1]; Ruwan T. Kurulugama[2]; Joseph C. Meeuwsen[1]; Bill Russ[2]; *[1]Agilent Technologies, CORVALLIS, OR; [2]Agilent Technologies, Santa Clara, CA*

TP 153 **Comparison of Gas Phase Fragmentation Behaviors of Nuclear Fuel Cycle Ligands in Lanthanide and Americium Metal Ligand**; JungSoo Kim[1]; Christopher A. Zarzana[1]; Brittany D. M. Hodges[1]; Corey D. Pilgrim[1]; *[1]Idaho National Laboratory, Idaho Falls, ID*

TP 154 **Electron Energy vs Density Effects in Peptide Cation-Electron Reactions: Proposed Alternative Fragmentation Mechanisms and Unexpected Observations**; Steven A. DeFiglia[1]; Neven N. Mikawy[1]; Teresa Lee[1]; Kristina Håkansson[1]; *[1]University of Michigan Department of Chemistry, Ann Arbor, MI*

TP 155 **Preliminary Implementation of a Xenon Reagent for Negative Electron Transfer Dissociation on Orbitrap Tribrid™ Systems**; Keaton L Mertz[1]; Daniel J Nesbitt[1]; Joshua J Coon[1, 2, 3, 4]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Morgridge Institute for Research, Madison, WI; [4]National Center for Quantitative Biology of Complex Systems, Madison, WI*

TP 156 **Ion Mobility Separation by means of Space Charge in Accumulation Regions with high concentrations**; Amirreza Tootchi[1]; Viraj D Gandhi[1, 2]; Farah Mubas-Sirah[1]; Carlos Larriba-Andaluz[1]; *[1]Indiana University Purdue University Indianapolis, Indianapolis, IN; [2]Purdue University, West Lafayette, IN*

FUNDAMENTALS: NATIVE MS
157-173

TP 157 **Native LC-MS Method Development for Characterization of Biologics on Orbitrap Eclipse Coupled with Acquity Premier UPLC**; Zhihao Yu[1]; Jacob Furlon[1]; Zhili Li[1]; *[1]Insmed, Bridgewater, NJ*

TP 158 **Native Top-Down Mass Spectrometry for Characterizing Sarcomeric Proteins Directly from Cardiac Tissue Lysate**; Brad Li[1]; Emily A Chapman[2]; Kevin M Buck[2]; Hsin-Ju Chan[2]; Boris Krichel[2]; David S Roberts[2]; Ying Ge[2, 3, 4]; *[1]University of Wisconsin-Madison, Department of Biochemistry, Madison, WI; [2]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [3]University of Wisconsin-Madison, Department of Cell and Regenerative Biology, Madison, WI; [4]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*

TP 159 **Measuring Effects of Biochemically Relevant Salts on Protein Stability and Conformation using Native Mass Spectrometry**; Katherine J Lee[1]; Jacob S Jordan[1]; Evan R Williams[1]; *[1]University of California, Berkeley, Berkeley, CA*

TP 160 **Affinity Painting of Membrane Protein-Lipid Interactions with Native Mass Spectrometry** ; Farhana Afrin Mohona[1]; Hiruni S. Jayasekera[1]; Megan Ewbank[1]; Michael Marty[1]; *[1]University of Arizona, Tucson, AZ*

TP 161 **Direct Analysis of SEC Fractionated E. coli Protein Complexes using Matrix-Landing Mass Spectrometry**; Noah M Lancaster[1, 2]; Austin Z Salome[1, 2]; Drew Jordahl[2]; Colin Hemme[3, 4]; Keaton L Mertz[1]; Mitchell D Probasco[4]; Erin L Mettert[2]; Patricia J Kiley[2]; Michael S Westphall[2, 5]; Scott T Quarmby[2, 5]; Timothy Grant[3, 4]; Joshua J Coon[1, 2, 4, 5]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [2]University of Wisconsin-Madison, Department of Biomolecular Chemistry, Madison, WI; [3]University of Wisconsin-Madison, Department of Biochemistry, Madison, WI; [4]Morgridge Institute for Research, Madison, WI; [5]National Center for Quantitative Biology of Complex Systems, Madison, WI*

TP 162 **Exploring cryo-electron microscopy compatible matrices for room temperature soft landing of macromolecules**; Drew Jordahl[1]; Austin Z Salome[1, 2]; Colin Hemme[3, 4]; Keaton L Mertz[1, 2]; Mitchell D Probasco[4]; Michael S Westphall[1, 5]; Scott T Quarmby[1, 5]; Timothy Grant[3, 4]; Joshua J Coon[1, 2, 4, 5]; *[1]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Department of Biochemistry, University of Wisconsin-Madison, Madison, WI; [4]Morgridge Institute for Research, Madison, WI; [5]National Center for Quantitative Biology of Complex Systems, Madison, WI*

TP 163 **Monitoring Effects of Nonvolatile Buffers on Assembly of Protein Complexes Using Native Mass Spectrometry and Ultraviolet Photodissociation**; Hanlin Ren[1]; Jennifer S. Brodbelt[1]; *[1]Department of Chemistry, University of Texas at Austin, Austin, TX*

TP 164 **Modeling the efficiency of collisional energy transfer and activation for native protein ions**; Austin W Green[1]; Samantha Shepherd[1]; Ruwan Kurulugama[2]; Kenneth Newton[1]; James Prell[1]; *[1]University of Oregon, Eugene, OR; [2]Agilent Technologies, Santa Clara, CA*

TP 165 **Direct Measurement of Binding Affinities of Weak Protein-Protein Interactions via Submicron Emitters and Native Mass Spectrometry**; Chae Kyung Jeon[1]; Emily G Sweeney[1]; Michael J Harms[1]; Karen Guillemin[1]; James S Prell[1]; *[1]University of Oregon, Eugene, OR*

TP 166 **Mechanistic insights into slow mixing in SLOMO-nMS**; Simar K. Dhillon[1]; Duong T. Bui[1]; Elena N. Kitova[1]; Lara K. Mahal[1]; Morris R. Flynn[1]; John S. Klassen[1]; *[1]University of Alberta, Edmonton, AB*

TP 167 **Elusive Protein–Glycosphingolipid Interactions Revealed by Membrane Anchor-Assisted (MEAN) Native Mass Spectrometry**; James W. Favell[1]; Duong T. Bui[1]; Jianing Li[1]; Ling Han[1]; Elena N. Kitova[1]; Edward N. Schmidt[1]; Pavel I. Kitov[1]; Lara K. Mahal[1]; Yves St-Pierre[2]; Matthew S. Macauley[1, 3]; John S. Klassen[1]; *[1]Department of Chemistry, University of Alberta, Edmonton, AB; [2]INRS-Institut Armand-Frappier, Laval, QC; [3]Department of Medical Microbiology and Immunology, University of Alberta, Edmonton, AB*

TP 168 **A Multidimensional Native Separation for the Online Analysis of Endogenous Protein Complexes from Human Heart Tissue**; Matthew S Fischer[1]; Holden T Rogers[1]; Emily A Chapman[2]; Boris Krichel[3, 4]; Eli J Larson[2]; Zhan Gao[3]; Andrew J Alpert[5]; Ying Ge[2, 3, 6]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [2]University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin; [3]University of Wisconsin-Madison, Department of Cell and Regenerative Biology, Madison, WI; [4]School of Life Sciences, University of Siegen, Siegen, Germany; [5]PolyLC Inc, Columbia, MD; [6]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*

TP 169 **Mapping protein structure stability for native mass spectrometry with vibrating sharp-edge spray ionization.**; Mst Nigar Sultana[1]; Vikum Dewasurendra[2]; Matthew Johnson[1]; Sultan Mahmud[3]; Mohammad Rahman[3]; Stephen Valentine[3]; Peng Li[3]; *[1]West Virgina University, Morgantown, WV; [2]West Virginia University, Morgantown, WV; [3]West Virginia University- C. Eugene Bennett Department of Chemistry, Morgantown, WV*

TP 170 **Native and native top-down mass spectrometry analysis of endogenous membrane proteins and their bound ligands directly from membranes**; Wonhyeuk Jung[1]; Aniruddha Panda[2]; Kallol Gupta[2]; *[1]Yale University, New Haven, CT; [2]Yale University, West Haven, CT*

TP 171 **On the “Freeze-Drying” [1] of Protein Solution Structures in the Absence of Solvent: Rugged Energy Landscape and Glass-Like Behavior**; Christian Bleiholder[1]; Tyler C. C Cropley[1]; Fanny C Liu[1]; Mengqi Chai[2]; Thais Pedrete[1]; Jusung Lee[1]; *[1]Florida State University, Tallahassee, FL; [2]Washington University in Saint Louis, St. Louis, MO*

TP 172 **Deep Ultraviolet and Infrared Laser Ablation of Carbonic Anhydrase II**; Neda Feizi[1]; Kadeem O Hayes[2]; Blessing Chisom Egbejiogu[2]; Kelcey B. Hines[2]; Kermit K. Murray[2]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX; [2]Louisiana State University, Baton Rouge, LA*

TP 173 **Cryogenic Soft Landing Improves Structural Preservation of Protein Complexes**; Austin Z Salome[1, 2]; Kenneth W Lee[2]; Colin Hemme[3, 4]; Michael S Westphall[2, 5]; Keaton L Mertz[1, 2]; Mitchell D Probasco[4]; Scott T Quarmby[2, 5]; Timothy Grant[3, 4]; Joshua J Coon[1, 2, 4, 5]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Department of Biochemistry, University of Wisconsin-Madison, Madison, WI; [4]Morgridge Institute for Research, Madison, WI; [5]National Center for Quantitative Biology of Complex Systems, Madison, WI*

HIGH THROUGHPUT MS I
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TP 174 **Determination of binding affinity with Rapid Equilibrium Dialysis (RED) and LC-MS**; Bryan Choi[1]; Calvin Han[1]; Jonathan LaRochelle[1]; Damian Houde[1]; *[1]Relay Therapeutics, Cambridge, MA*

TP 175 **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 176 **High-throughput MS-based cholesterol quantitation assay for Niemann-Pick Disease type C (NPC)**; Yuhong Fang[1]; Yi-Han Lin[1]; Maya L. Gosztyla[1]; Edward Zhu[1]; Abhijeet Kapoor[1]; Andrés E. Dulcey[1]; Daniel C. Talley[1]; Mark J. Henderson[1]; Xin Hu[1]; Wei Zheng[1]; Anton Simeonov[1]; Juan J. Marugan[1]; Christopher A LeClair[1]; Bolormaa Baljinnyam[1]; Dingyin Tao[1]; *[1]National Center for Advancing Translational Sciences, NIH, Rockville, MD*

TP 177 **High-throughput Characterization of Therapeutic Proteins by Peptide Mapping Using Ultra-High Pressure Liquid Chromatography (>1,000 bar) Mass Spectrometry**; Andrew B. Dykstra[1]; Prashant N. Jethva[1]; Daniel W. Woodall[1]; Pavel V. Bondarenko[1]; *[1]Amgen, Thousand Oaks, CA*

TP 178 **High-throughput Mass Spectrometry - Based Detec--tion of Deamination Activity of ADAR1 without Prior Separation**; Yating Wang[1]; Travis Pemberton[1]; Ping Zhang[2]; Iyoncy Rodrigo[2]; Zhigang Wang[1]; *[1]Bristol Myers Squibb, Cambridge, MA; [2]Bristol Myers Squibb, Lawrenceville, NJ*

TP 179 **Pushing the limits of uncompromised high-throughput HCP profiling with utmost speed and sensitivity**; Kristina Srzentic[1]; Kai Scheffler[2]; Florian Bonn[3]; Tabiwang Arrey[3]; Nicolaie Eugen Damoc[3]; Ales Holfeld[1]; *[1]Thermo Fisher Scientific, Reinach, Switzerland; [2]Thermo Fisher Scientific, Germering, Germany; [3]Thermo Fisher Scientific, Bremen, Germany*

TP 180 **Rapid determination of four anions in urine**; Xiao Luo[1]; Yanjian Wan[2]; Liuqing Zhao[3]; Zong Yang[3]; Bingjie Liu[3]; Lihai Guo[3]; *[1]Key Laboratory of Environment and Health, Tongji Medical College, Huazhong University of Science and Technology, Wuhan, China; [2]Center for Public Health Laboratory Service, Institute of Environmental Health, Wuhan Centers for Disease Control & Prevention, Wuhan, China; [3]SCIEX Asia Pacific Application Support Center,, Shanghai, China*

TP 181 **OPSI-MS: System integration for high-throughput bioanalysis**; Manan Luthra[1]; Savannah Wood[1]; Nate Hoxie[1]; Vijay Veerisetty[1]; Anthony Garrison[1]; Pranav Bende[1]; John Janiszewski[1]; Jonathan Shrimp[1]; Meghav Verma[1]; Sam Michael[1]; Matthew D Hall[1]; Peter Kovarik[2]; Tom Covey[2]; Chang Liu[2]; *[1]NIH/NCATS, Rockville, Maryland; [2]SCIEX, Concord, ON*

TP 182 **High-throughput affinity selection-mass spectrometry system using novel nanoparticle ferrimagnetic beads**; Richard B. Van Breemen[1]; Jenna Miller[2]; Nate Hoxie[2]; Meghav Verma[2]; Michael Ronzetti[2]; John Janiszewski[2]; Bolormaa Baljinnyam[2]; Jonathan Shrimp[2]; Anton Simeonov[2]; Sam Michael[2]; Matthew D Hall[2]; Daniel Simchuk[1]; Jianli Zhao[3]; Sasikumar PlIlai[4]; Babu Purkayastha[4]; Peter Kovarik[5]; Tom Covey[5]; Chang Liu[5]; *[1]Oregon State University, Corvallis, OR; [2]National Center for Advancing Translational Sciences (NCATS), Rockville, MD; [3]Phenomenex, Torrance, CA; [4]Sciex, Framingham, MA; [5]SCIEX, Concord, ON*

TP 183 **Automatic cleaning in Acoustic Ejection Mass Spectrometry: Enhancing the system robustness for large-scale high-throughput analysis of complex samples**; Heguang Ji[1]; Xuejiao Yin[1]; Wan Ee Ang[1]; Abdullah Bin Rawshan[1]; Susan Gay[1]; Jing Ma[1]; Chiu Cheong Aw[1]; Parikshit Gokhale[2]; Chang Liu[2]; *[1]SCIEX, Singapore, Singapore; [2]SCIEX, Concord, ON*

TP 184 **Development of high throughput isotope dilution protocols for I.DOT/OPSI-MS for determination of nitrification and mineralization rates in soil**; John F. Cahill[1]; Vilmos Kertez[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN*

TP 185 **A faster scanning DIA approach for high throughput quantitative proteomics**; Anjali Chelur[1]; Stephen Tate[1]; Claudia Alvarez[1]; Gordana Ivosev[1]; Nic G Bloomfield[1]; *[1]SCIEX, Concord, ON*

TP 186 **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[1]; Andrew Porter[1]; Pawel Palmowski[1]; Quentin M Anstee[1]; Ann Daly[1]; Matthias Trost[1]; *[1]Newcastle University, Newcastle upon Tyne, United Kingdom*

TP 187 **A complete and automated end-to-end sample preparation strategy for high-throughput and standardized proteomics with high sensitivity**; Magnus Huusfeldt[1]; Hope Cabalo Zisco[1]; Dorte B Bekker-Jensen[1]; Nicolai H Bache[1]; *[1]Evosep, Odense, Denmark*

TP 188 **Inter-laboratory assessment of standardized and fully automated, sample preparation workflows integrated with EvosepOne**; Andrea Ellero[1, 2]; Camilla O. Kuhl[3]; Joel M. Vej-Nielsen[3]; Adele Nel[1, 2]; Anne Katrine Ravno[3]; Ireshyn S Govender[1, 4]; Previn Niacker[1, 4]; Stoyan Stoychev[3, 5]; Dorte B. Bekker-Jensen[3]; Nicolai Bache[3]; Justin Jordaan[1]; *[1]ReSyn Biosciences, Pretoria, South Africa; [2]University of Pretoria, Pretoria, South Africa; [3]Evosep, Odense, Denmark; [4]Council for Scientific and Industrial research, Pretoria, South Africa; [5]ReSyn BioSciences, Johannesburg, South Africa*

TP 189 **Next-generation Acoustic Ejection Mass Spectrometry: A fully automated platform for high-throughput sample analysis**; Jacob Watson McCabe[1]; Aaron Stella[1]; Anuja Bhalkikar[1]; Heidi D Paolieri[2]; Marisa A Spence[2]; Sarah Simons[2]; Han Joo Lee[1]; *[1]SCIEX, USA, Framingham, MASSACHUSETTS; [2]Beckman Coulter Life Sciences, Indianapolis, IN*

TP 190 **A high-throughput, compound agnostic target engagement assay for covalent inhibitors of G12C KRAS using acoustic droplet ejection mass spectrometry**; Michelle Robinson[1]; Rajesh Desai[1]; Nicolas Solban[2]; Weixun Wang[1]; *[1]Merck & Co., Inc., West Point, PA; [2]Merck, Boston, MA*

TP 191 **Affinity-Selection Mass Spectrometry (MagMASS) for the Discovery of Ligands for the SHIP1 protein involved in Alzheimer's Disease**; Daniel D Simchuk[1, 2]; Andrew D Mesecar[3]; Adam K Hamdani[3]; Richard Van Breemen[1, 2]; *[1]Oregon State University, Corvallis, OR; [2]Linus Pauling Institute, Oregon State University, Corvallis, OR; [3]Department of Biochemistry, Purdue University, West Lafayette, IN*

TP 192 **An affinity selection-mass spectrometry screen (ASMS) for identifying novel tyrosine kinase 2 (TYK2) allosteric Inhibitors**; Reza Nemati Josheghani[1]; Naifu Zhang[1]; Ronghai Cheng[1]; Daniel Tekverk[1]; Howard Jones[1]; Martin Himmelbauer[1]; *[1]Biogen, Cambridge, MA*

TP 193 **High-throughput LC-MS quantification of secreted delta-hemolysin toxin from clinical S. aureus isolates**; Ioana Clotea[1]; Magdalena Podkowik[2]; Bo Shopsin[2, 3]; Beatrix Ueberheide[1]; *[1]Proteomics Laboratory, Division of Advanced Research Technologies, New York University Grossman School of Medicine, New York, NY; [2]Department of Medicine, Division of Infectious Diseases, NYU Grossman School of Medicine, New York, NY; [3]Department of Microbiology, NYU Grossman School of Medicine, New York, NY*

TP 194 **Mass spectrometry-based screening platform for transition metal nanoparticle catalysis**; Tingyuan Yang[1]; Nilotpal Kapuria[2]; Baixu Zhu[3]; Xingchen Ye[2]; Xin Yan[4]; *[1]TAMU, College Station, TX; [2]Indiana University Bloomington, Bloomington, IN; [3]Indiana University, Bloomington, IN; [4]Texas A&M University, College Station, TX*

TP 195 **Ultra-fast Multiplexed LC/MS/MS Using Newly Designed Online SPE Column for the Simultaneous Analysis of Steroid Hormones in Human Serum**; Eishi IMOTO[1]; Vikki JOHNSON[2]; Logan MILLER[1]; Toshiya MATSUBARA[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]Shimadzu scientific instruments, Carlsbad, CA*

TP 196 **Development of High-throughput LC-MS/MS Method for UV Stability Study**; Xiaodong Liu; *Corteva Agriscience, Indianapolis, IN*

TP 197 **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[1]; Trevor N. Clark[2]; Adam M. King[3]; Lee A Gethings[3]; David Heywood[3]; Roger G. Linington[1]; *[1]Simon Fraser University, Burnaby, BC; [2]University of Prince Edward Island, Charlottetown, PEI; [3]Waters Corporation, Wilmslow, United Kingdom*

TP 198 **MetwareBio: Pioneering Mass Spectrometry Innovations for Advanced Metabolomics, Proteomics, and Cloud-Based Research Excellence**; James Dong; *Metware Biotechnology Inc., Woburn*

IMAGING MS: INSTRUMENTATION
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TP 199 **BeamMap: A multi-modal mass spectrometry and electron microscopy imaging instrument on the single-cell scale**; John Sentmanat[1]; Mazdak Taghioskoui[2]; Peter Kottke[1]; Andrei Fedorov[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Trace Matters Scientific, Bethesda, MD*

TP 200 **Matrix Assisted Laser Desorption Ionisation-Immunohistochemistry (MALDI-IHC) Mass Spectrometry Imaging of Human Tonsil using an Entry-Level Benchtop MALDI-TOF Platform**; Caroline Jones[1]; Simona Salivo[1]; Matthew Openshaw[1]; *[1]Kratos Analytical Ltd., Manchester, United Kingdom*

TP 201 **High-Spatial-Resolution Mass Spectrometry Imaging of Phospholipid Biosynthesis-Impaired Mouse Testis via Tapping-Mode Scanning Probe Electrospray Ionization**; Yoichi Otsuka[1]; Maki Okada[2]; Tomomi Hashidate-Yoshida[3]; Katsuyuki Nagata[3]; Makoto Yamada[4]; Motohito Goto[5]; Mengze Sun[2]; Hideo Shindou[3, 6]; Michisato Toyoda[2]; *[1]Osaka University, Toyonaka, Japan; [2]Osaka University, Toyonaka, Japan; [3]National Center for Global Health and Medicine, Shinjuku, Japan; [4]Shimadzu Corporation, Nakagyo-ku, Japan; [5]Central Institute for Experimental Animals, Kawasaki, Japan; [6]The University of Tokyo, Bunkyo-ku, Japan*

TP 202 **Optimisation on the new generation of microscope mode secondary ion mass spectrometry imaging**; Yifeng Jia[1]; Elena Castellani[1, 2]; Felicia Green[2]; Kieran Cheung[3]; Josh Featherstone[3]; Michael Burt[3]; Mark Brouard[3]; Zoltan Takats[2]; *[1]Department of Chemistry, University of Oxford,, Oxford, United Kingdom; [2]The Rosalind Franklin Institute, Oxford, United Kingdom; [3]Department of Chemistry, University of Oxford, Oxford, United Kingdom*

TP 203 **Characterization of a new MALDI-TOF axial benchtop instrument for MALDI Imaging applications**; Michael Easterling[1]; Sebastian Boehm[2]; Christoph Nordmann[2]; Andreas Haase[2]; Janina Oetjen[2]; Jan Hendrik Kobarg[2]; Tobias Boskamp[2]; Ulrike Schweiger Hufnagel[2]; Jens Christmann[3]; Andrea Tannapfel[3]; Andree Schuster[2]; Katherine Stumpo[1]; Jens Hoehndorf[2]; *[1]Bruker Scientific, 40 Manning Road, Billerica, MA; [2]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; [3]Institute for Pathology, Ruhr-University Bochum, Bürkle-de-la-Camp-Platz 1, 44789 Bochum, Germany*

TP 204 **An Automated System for High-throughput Nanospray Desorption Electrospray Ionization Mass Spectrometry Imaging**; Lixue Jiang[1]; Emerson Hernly[1]; Benjamin Cerjan[1]; Julia Laskin[1]; *[1]Purdue University Department of Chemistry, West Lafayette, IN*

TP 205 **Different approaches to 3D Imaging Analysis for observing molecular collision and/or dissociation products**; Joshua Featherstone[1]; Max McCrea[1]; Matt Strutton[1]; Kieran Cheung[1]; Joseph McManus[1]; Chow-shing Lam[1]; Yifeng Jia[1]; Elena Castellani[1, 2]; Felicia Green[2]; Mark Brouard[1]; *[1]University of Oxford, Oxford, United Kingdom; [2]Rosalind Franklin Institute, Didcot, United Kingdom*

TP 206 **Improvements in fast mass microscopy for biomedical applications**; Aljoscha Körber[1]; Edith Sandström[1]; Kasper Krijnen[1]; Frans Giskes[1]; Pascal Huysmans[1]; Paul Laeven[1]; Ian G. M. Anthony[1]; Ron M. A. Heeren[1]; *[1]Maastricht University, Maastricht, Netherlands*

TP 207 **IR-MALDESI Coupled to a Trapped Ion Mobility Spectrometry and Time-of-Flight Mass Spectrometer**; Kevan T Knizner[1]; Joshua L. Fischer[2]; Mary F Wang[1]; Alexandria L. Sohn[1]; Russell R Kibbe[1]; Daniel C Castro[2]; Jeremy L Norris[2]; David C. Muddiman[1]; *[1]North Carolina State University, Raleigh, NC; [2]Bruker Daltonics, Billerica, MA*

TP 208 **Comparison of instrumental synchronization modes in mass spectrometric imaging using Orbitrap mass analyzers**; Karl Christian Schäfer[1]; Lars Liebschwager[1]; Kerstin Strupat[2]; Bernhard Spengler[1, 3]; *[1]Transmit GmbH, Giessen, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Justus Liebig University, Giessen, Germany*

IMAGING MS: PHARMACEUTICALS, METABOLITES, LIPIDS, AND GLYCANS II
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TP 209 **Targeted DESI Imaging MS of Drug Distribution and Drug-Induced Liver Injury (DILI) Metabolites from Methapyrilene in the Male Wistar Rat**; Anthony J Midey[1]; Steven K Lai[1]; Ian D Wilson[2]; Robert S Plumb[1]; Roy Martin[1]; *[1]Waters, Milford, MA; [2]Imperial College London, London, United Kingdom*

TP 210 **A lipidomics approach reveals novel lipid changes in skeletal muscles due to muscle hypertrophy and atrophy**; Naoko GOTO-INOUE; *Nihon University, Fujisawa, Japan*

TP 211 **Multimodal mass spectrometry imaging reveals biodistributions and biochemical effects of polymeric nanomaterial therapeutic delivery systems**; Jeerapat Doungchawee[1]; Dheeraj K. Agrohia[2]; Teerapong Jantarat[2];

Richard W. Vachet[2]; *[1]University of Masssachusetts Amherst, amherst, MA; [2]University of Massachusetts Amherst, Amherst, MA*

TP 212 **Enhancing detection and metabolite annotations in MS imaging using on-tissue chemical derivatization and ion mobility with in-silico prediction of derivatization** ; Dušan Veličković[1]; Kevin Zemaitis[1]; Aiko Barsch[2]; Arne Behrens[2]; Nannan Tao[3]; Nikolas Kessler[2]; Sofie Weinkouff[2]; Christopher Anderton[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Bruker Daltonics, Billerica, MA*

TP 213 **Spatial mapping of N-glycan distributions in a mouse model of primary graft dysfunction post-lung transplantation**; Ariana E Stratton[1]; Hassan H Moussa[2]; Carl Atkinson[2]; Boone M. Prentice[1]; *[1]University of Florida Department of Chemistry, Gainesville, FL; [2]University of Florida, Department of Medicine, Gainesville, FL*

TP 214 **Imaging Mass Spectrometry Analysis of Mouse Choroid Plexus**; Michelle Reyzer[1]; Angela Wang[1]; Audra M. Judd[1]; Neil Dani[1]; Richard M. Caprioli[1]; *[1]Vanderbilt University, Nashville, TN*

TP 215 **MALDI imaging of glucose in tissue sections by derivatization with betaine aldehyde versus NDEC matrix approach**; Anna Bodzon-Kulakowska[1]; Paulina Kret[1]; Przemysław Mielczarek[1]; Piotr Suder[1]; *[1]AGH Univeristy of Krakow, Krakow, Poland*

TP 216 **Isomer and Isobar Spatial Traumatic Brain Injury Lipidomics with Desorption Electrospray Ionization Cyclic Ion Mobility Mass Spectrometry Imaging**; Dmitry Leontyev[1]; Hernando Olivos[2]; Bindesh Shrestha[2]; Pooja M Datta Roy[1, 3]; Michelle C. LaPlaca[1, 3]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Waters Corporation, Milford, MA; [3]Emory University, Atlanta, GA*

TP 217 **Spatial mapping of plant specialized metabolites using imaging mass spectrometry**; Tetsuya Mori[1]; Noriko Kamiya Takeda[1]; Mai Uzaki[1]; Tomoko Nishizawa[1]; Kiminori Toyooka[1]; Masami Hirai[1]; *[1]RIKEN CSRS, Yokohama, Japan*

TP 218 **Unraveling the effects of eribulin pretreatment on docetaxel distribution in tumour xenografts using AP MALDI Mass Spectrometry Imaging**; Alice Passoni[1]; Stefano Mauro Carabellese[1]; Cristina Matteo[1]; Marta Cancelliere[1]; Alessia Lanno[1]; Ugo Cavallaro[2]; Salvatore Lorenzo Renne[3]; Lavinia Morosi[3]; Renzo Bagnati[1]; Massimo Zucchetti[1]; Enrico Davoli[1]; Roberta Frapolli[1]; *[1]Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy; [2]European Institute of Oncology IRCCS, Milan, Italy; [3]IRCCS - Humanitas Research Hospital, Rozzano, Italy*

TP 219 **Harnessing the Power of MSI to Improve BASF Formulation and Product Development of Insecticides, Surfactants, and Polymers**; Alanna R Condren[1]; Steven A. DeFiglia[2]; Neven N. Mikawy[2]; James Austin[3]; Kristina Hakansson[2]; Shawn Zhao[1]; *[1]BASF Corporation, Wyandotte, MI; [2]University of Michigan Department of Chemistry, Ann Arbor, MI; [3]BASF Corporation, Research Triangle Park, NC*

TP 220 **Spatially Resolved Analysis of glycosaminoglycans (GAGs) Utilising Trapped Ion Mobility Spectrometry (TIMS)**; Anthony J Devlin[1]; C. Logan Mackay[1]; Christopher A Wootton[2]; Felicia Green[1, 3]; Zoltan Takats[1, 4]; *[1]Rosalind Franklin Institute, Didcot, United Kingdom; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [3]University of Oxford, Oxford, United Kingdom; [4]Imperial College London, London, United Kingdom*

TP 221 **Label-Free High-Resolution Molecular Imaging of Sex Steroid Hormones in Zebrafish by Water Cluster Secondary Ion Mass Spectrometry (Cluster SIMS)**; Naoko Sano[1]; Elkan Lau[2]; Johanna Von Gerichten[2]; Kate McHardy[3]; Paul Blenkinsopp[3]; Maya Al Sid Cheikh[2]; Melanie Bailey[2]; *[1]Ionoptika Ltd, Chandlers Ford, United Kingdom; [2]University of Surrey, School of Chemistry and Chemical Engineering, Guildford, United Kingdom; [3]Ionoptika Ltd, Eastleigh, United Kingdom*

TP 222 **The Effect of Thrombin-Sensitive Platelet-like Particles on the Liver N-Linked Glycome**; Seth M. Eisenberg[1]; Sanika Pandit[2, 3]; Ashley Brown[2, 3]; David C. Muddiman[1]; *[1]FTMS Laboratory for Human Health Research, Raleigh, NC; [2]Joint Department of Biomedical Engineering, North Carolina State University and University of North Carolina-Chapel Hill, Raleigh, NC; [3]Comparative Medicine Institute, Raleigh, NC*

TP 223 **Multimodal Mass Spectrometry Imaging of an Osteosarcoma Multicellular Tumour Spheroid Model to Investigate Drug Induced Response**; Sophie M Pearce[1]; Neil A Cross[1]; David P Smith[1]; Malcolm R Clench[1]; Lucy E Flint[2]; Gregory Hamm[2]; Richard Goodwin[2]; James I. Langridge[3]; Emmanuelle Claude[3]; Laura M Cole[1]; *[1]Centre for Mass Spectrometry Imaging, Biomolecular Sciences Research Centre, Sheffield Hallam University, Sheffield, United Kingdom; [2]AstraZeneca, Cambridge, United Kingdom; [3]Waters Corporation, Wilmslow, United Kingdom*

TP 224 **MALDI-MS imaging reveals spatially-localized differences in Ferroptosis-associated lipids in ileum after total body irradiation (TBI)**; L.J. Sparvero[1]; Hua Tian[1]; Yulia Tyurina[1]; Michael W Epperly[1]; Joel S. Greenberger[1]; Diane K. Luci[2]; Adam Yasgar[2]; Sandeep Rana[2]; Anton Simeonov[2]; Alexey V. Zakharov[2]; Ganesha Rai[2]; Hülya Bayır[3]; Valerian E. Kagan[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]National Center for Advancing Translational Sciences (NCATS), Rockville, MD; [3]Columbia University Irving Medical Center, New York, NY*

TP 225 **Evaluating D-Amino Acid Influence on Biofilms in Pseudomonas aeruginosa Lung Infections Under Cystic Fibrosis Conditions through Mass Spectrometry Imaging**; Joenisse M Rosado-Rosa[1]; Dharmeshkumar Parmar[1]; Joshua D Shrout[2]; Paul W Bohn[2]; Jonathan V Sweedler[1]; *[1]University of Illinois Urbana-Champaign, Urbana, IL; [2]University of Notre Dame, Notre Dame, IN*

TP 226 **MALDI IMS of pharmaceutical tablets at 10-µm pixel size without laser oversampling: workflow and surface quality considerations**; Alvaro Santos-Neto[1, 2]; Georgia Charkoftaki[1]; Athina Lisgara[1]; Reza Aalizadeh[1]; Scott Pennino[3]; John Smoliga[3]; Michelle Raikes[3]; Nina Gonnella[3]; Michael Becker[4]; Vladimir V. Papov Jr. [3]; Vasilis Vasiliou[1]; *[1]Department of Environmental Health Sciences, Yale School of Public Health, Yale University, New Haven, Connecticut; [2]São Carlos Institute of Chemistry, University of São Paulo, São Carlos 13566-590, SP, Brazil, Brazil; [3]Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, Connecticut; [4]Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach/Riss, Germany*

TP 227 **Mapping nutrient movement, developmental morphogen gradients and electromotive drug delivery with MALDI-TOF Imaging Mass Spectrometry**; Felix Grun[1]; Agatha Kliman[2]; Yi Xi Wu[2]; Matthew Chang[3]; *[1]University of California Irvine, Irvine, CA; [2]University of California, Irvine, Irvine, CA; [3]Woodbridge HS, Irvine, California*

TP 228 **Optimization of MALDI-MSI detecting branched-chain amino acids (BCAAs) in Gut-Brain Axis**; Sydni L Chaney[1]; Bandana Bera[2]; Brendan Prideaux[2]; *[1]The University of Texas Medical Branch, Galveston, TX; [2]University of Texas Medical Branch at Galveston, Galveston, TX*

TP 229 **Metabolic alterations of Staphylococcus aureus murine bone infection visualized via MALDI Imaging Mass Spectrometry**; Lauren Emmerson[1, 2]; Christopher J. Good[1, 3]; Madeline E Colley[1, 4]; Ali Zahraei[1, 5]; Lukasz Migas[1, 6]; Raf Van De Plas[1, 4, 6]; James E. Cassat[7, 8, 9, 10]; Jeffrey M Spraggins[1, 2, 3, 4, 5, 7, 10]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Chemical and Physical Biology Program, Vanderbilt University, Nashville, Tennessee; [3]Department of Chemistry, Vanderbilt University, Nashville, TN; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN; [5]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [6]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [7]Department of Pathology, Microbiology, and Immunology, Vanderbilt University*

Medical Center, Nashville, TN; [8]Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; [9]Department of Biomedical Engineering, Vanderbilt University, Nashville, Tennessee; [10]Vanderbilt Institute for Infection, Immunology and Inflammation, Vanderbilt University School of Medicine, Nashville, Tennessee

TP 230 **Analysis and comparison of matched FFPE and fresh frozen tissue by multimodal mass spectrometry imaging**; Rory Thomas Steven[1]; Angeliki Christakopoulou[1]; Bin Yan[1]; Ariadna Gonzalez[1]; Josephine Bunch[1, 2]; *[1]National Physical Laboratory, London, United Kingdom; [2]Imperial College London, London, United Kingdom*

TP 231 **MALDI Mass Spectrometry Imaging of Aspirin Metabolites and Prostaglandins to Investigate Inflammatory Pathways in Breast Cancer**; Taehun Hahm[1, 2]; Michael T McMahon[1, 3]; Dalton Brown[1, 2]; Cole Johnson[1, 2]; Caitlin M. Tressler[1, 2]; Kristine Glunde[1, 2]; *[1]Johns Hopkins University School of Medicine, Baltimore city, MD; [2]Johns Hopkins Applied Imaging Mass Spectrometry (AIMS) Core, Baltimore city, MD; [3]Kennedy Krieger Institute, Baltimore city, MD*

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TP 232 **Applications of all-ion fragmentation for sensitive imaging of esterified fatty acids**; Maans Ekeloef[1]; Elena Buglakova[1]; Marteinn Snaebjoernsson[2]; Michaela Schwaiger-Haber[3]; Gary J. Patti[3]; Almut Schultze[2]; Theodore Alexandrov[1]; *[1]EMBL, Heidelberg, Germany; [2]DKFZ German Cancer Research Center, Heidelberg, Germany; [3]Washington University in Saint Louis, St. Louis, MO*

TP 233 **Linking MALDI MSI and functional proteomics from heterogeneous tissues: a pixel-by-pixel shotgun spatial proteomic approach**; Christopher Kune[1]; Matthieu Hodeige[1]; Maximilien Fleron[2]; Dominique Baiwir[2]; Nor Eddine Sounni[3]; Gauthier Eppe[1]; Gabriel Mazzucchelli[1, 2]; *[1]Mass Spectrometry Laboratory, MolSys Research Unit, University of Liege, Liege, Belgium; [2]GIGA Proteomics Facility, University of Liège, Liège, Belgium; [3]Laboratory of Tumor and Development Biology, GIGA-Cancer, University of Liege, Liege, Belgium*

TP 234 **Laser Photobleach Assisted Spatial Proteomics Method for Tissue Sampling in Zebrafish**; Julia Ekiert[1]; Beatriz Ibarra[1]; Ankur Saxena[2]; Yu Gao[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]University of Alabama Birmingham, Birmingham, Alabama*

TP 235 **Open source and scalable spatial reactomics workflow for high resolution mass spectrometry imaging**; Miao Yu[1]; Ron Korstanje[2]; Brian Hoffmann[2]; Tim Stodola[2]; Sheng Li[1]; Matt Mahoney[2]; Vivek Philip[2]; Paul Robson[1]; Nadia Rosenthal[2]; *[1]The jackson laboratory, Farmington, CT; [2]The Jackson Laboratory, Bar Harbor, ME*

TP 236 **Mass spectrometry imaging of the developing amphibian brain as a tool to discover molecular markers of neurodevelopment**; Rikke Poulsen[1, 2, 3]; Emma M. Field[2]; Haley Kuecks-Winger[2]; Angela M. Jackson[1]; David Goodlett[1, 2]; Martin Hansen[3]; Caren C. Helbing[2]; Helena Petrosova[1, 2]; *[1]University of Victoria Genome BC Proteomics Centre, Victoria, BC; [2]University of Victoria, Departmemt of Biochemistry and Microbiology, Victoria, BC; [3]Aarhus University, Department of Environmental Science, Roskilde, Denmark*

TP 237 **Untargeted Spatial Metabolomics and Spatial Proteomics on the Same Tissue Section**; Gregory W Vandergrift[1]; Marija Veličković[1]; Le Z Day[1]; Sarah M Williams[1]; Bindesh Shrestha[2]; Roy Martin[2]; Christopher R Anderton[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Waters Corporation, Milford, MA*

TP 238 **Deciphering the Three-Dimensional Biomolecular Distribution in the Alzheimer's Disease Brain: A Multiomic Approach Integrating Immunohistochemistry with MALDI MS Imaging**; Kelly H. Lu[1]; Hua Zhang[2]; Gargey B. Yagnik[3]; Mark J. Lim[3]; Kenneth J. Rothschild[3, 4]; Andrew J. Schneider[5, 6]; Luigi Puglielli[5, 6]; Lingjun Li[7, 8]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin; [2]University of Wisconsin-Madison School of Pharmacy, Madison, WI; [3]AmberGen Inc., Billerica, MA; [4]Boston University, Department of Physics and Photonics Center, Boston, MA; [5]University of Wisconsin-Madison, Department of Medicine, Madison, WI; [6]University of Wisconsin-Madison, Waisman Center, Madison, WI; [7]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [8]University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin*

TP 239 **Decoding Molecular Barcodes of Glomerular Cell Types Through Integrated MALDI IMS and Multiplexed Immunofluorescence Microscopy**; Allison B Esselman[1, 2]; Léonore Tideman[3]; Felipe A Moser[3]; Lukasz Migas[2, 3]; Katerina V Djambazova[2, 4]; Madeline E Colley[2, 5]; Ellie L Pingry[2, 4]; Nathan Heath Patterson[2, 5]; Melissa A Farrow[2, 5]; Haichun Yang[6, 7]; Agnes B Fogo[6, 7, 8, 9]; Mark DeCaestecker[8]; Raf Van De Plas[2, 3, 5]; Jeffrey M Spraggins[1, 2, 4, 5, 6]; *[1]Chemistry Department, Vanderbilt University, Nashville, TN; [2]Mass Spectrometry Research Center, Nashville, TN; [3]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [4]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [5]Department of Biochemistry, Vanderbilt University, Nashville, TN; [6]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; [7]Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; [8]Division of Nephrology and Hypertension, Vanderbilt University Medical Center, Nashville, TN; [9]Department of Medicine, Vanderbilt University Medical Center, Nashville, TN*

TP 240 **Coupled MALDI-IMS and Intact Glycoproteomics for Comprehensive Spatial Analysis in Mucinous Tumor Tissues**; Sarah C. Lowery[1]; Rachel Stubler[2]; Isabella Tran[1]; Keira E. Mahoney[1]; Georgia Charkoftaki[1]; Vasilis Vasiliou[1]; Richard R Drake[2]; Stacy A. Malaker[1]; *[1]Yale University, New Haven, CT; [2]Medical University of South Carolina, Charleston, SC*

TP 241 **A preliminary analysis towards the spatial proteomics landscapes of the chemo-refractory related high-grade serous ovarian cancer**; Linyuan Fan[1]; Haichao Zhou[1]; Yi Liu[2]; Yang Feng[1]; Guixue Hou[1]; Jianqing Zhu[2]; Siqi Liu[1, 3]; *[1]University of Chinese Academy of Sciences, Beijing, China; [2]Zhejiang Cancer Hospital, Hangzhou Institute of Medicine (HIM), Chinese Academy of Sciences, Hangzhou, China; [3]BGI-Shenzhen, Shenzhen, China*

TP 242 **Mapping Molecular Profiles to Cell Types and Neighborhoods through the Integration of MALDI IMS and CODEX Multiplexed IF**; Thai H Pham[1, 2]; Ellie L Pingry[1, 2]; Martin Dufresne[1, 3]; Lukasz Migas[1, 4]; Felipe A Moser[4]; Madeline E Colley[1, 3]; Angela R. S. Kruse[1, 2]; Melissa A. Farrow[1, 3]; Raf Van De Plas[1, 4]; Jeffrey M Spraggins[1, 2, 3, 5, 6]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, Tennessee; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Department of Chemistry, Vanderbilt University, Nashville, TN; [6]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN*

TP 243 **ToF-SIMS-based imaging of unsaturated fatty acyl chain in cell membranes via Pd-catalyzed deuteration**; Yooseong Jeong[1]; Dong-Kyu Lee[1]; *[1]College of Pharmacy, Chung-Ang University, Seoul, South Korea*

TP 244 **Mobility-Modulated Sequential Dissociation Analysis Enables Structural Lipidomics in Mass Spectrometry Imaging**; Yao Qian[1]; Zheng Ouyang[1]; Xiaoxiao Ma[2]; *[1]Tsinghua University, Beijing, China; [2]Tsinghua University, Beijing, China*

TP 245 **Exploring the differences in lipid composition of neurons between male and female mice using MALDI-IMS**; Cristina Huergo[1]; Laura De Las Heras-Garcia[2, 3, 4]; Jone

Razquin[3, 4, 5]; Cristina Miguelez[2, 3, 4]; Jose A Fernandez[1]; *[1]Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Leioa, Spain; [2]Dep of Pharmacology, University of the Basque Country (UPV/EHU), Leioa, Spain; [3]Biocruces Health Research Institute, Neurodegenerative diseases, Barakaldo, Spain; [4]Institut des Maladies Neurodegeneratives IMN, CNRS/University of Bordeaux, Bordeaux, France; [5]Pharmacology, University of the Basque Country (UPV/EHU), Leioa, Spain*

TP 246 **Combining Drug and Targeted Protein Imaging to Uncover Molecular Changes Associated with Cancer Treatment**; Erin H Seeley[1]; Catherine A Kita[2]; Gargey B. Yagnik[2]; Kenneth J. Rothschild[2, 3]; Mark J. Lim[2]; Rahul A. Sheth[4]; *[1]University of Texas at Austin, Austin, TX; [2]AmberGen Inc., Billerica, MA; [3]Boston University, Department of Physics and Photonics Center, Boston, MA; [4]MD Anderson Cancer Center, Houston, Texas*

TP 247 **Multiplexed targeted imaging of intact proteins in tissue by multi reflecting time of flight (MRT) MALDI-IHC**; Mark Towers[1]; Joel Keelor[2]; Gabriel Stefan Horkovics-Kovats[3]; Steven Pringle[1]; Joanne Ballantyne[1]; Lisa Reid[4]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]Hevesy György PhD School, Eötvös Loránd University, Budapest, Hungary; [4]Waters Corporation, Wilmslow, United Kingdom*

TP 248 **MS Imaging for Differential Neuropeptides and Neurotransmitters Colocalization in Cancer borealis Stomatogastric Nervous System Resulting from Food Intake**; Wenxin Wu[1]; Penghsuan Huang[1]; Haoran Zhang[1]; Angel E. Ibarra[1]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

TP 249 **Combined Spatially-Resolved Proteomics and Lipidomics Decipher the Interaction of Collagens and Lipids in Parchment Objects**; Antonia Malissa[1]; Manfred Schreiner[1, 2]; Martina Marchetti-Deschmann[1]; *[1]TU Wien, Vienna, Austria; [2]Academy of Fine Arts Vienna, Vienna, Austria*

TP 250 **Multimodal Multiplexed Approaches to Assess the Triple-Negative Breast Cancer Microenvironment Linked to Staging and Survival**; Jaclyn B. Dunne[1]; Heather Jensen-Smith[2]; Laura Spruill[1]; Taylor Hulahan[1]; Juliana Gonçalves[3]; Kristina Schwamborn[3]; Mark J. Lim[4]; Gargey B. Yagnik[4]; Kenneth J. Rothschild[4, 5]; Anand S. Mehta[1]; Richard R. Drake[1]; Graham Colditz[6]; Marvella E. Ford[1]; Peggi M. Angel[1]; *[1]Medical University of South Carolina, Charleston, SC; [2]University of Nebraska Medical Center, Omaha, NE; [3]Technical University of Munich (TUM), Munich, Germany; [4]AmberGen Inc, Billerica, MA; [5]Boston University, Department of Physics and Photonics Center, Boston, MA; [6]Washington University in Saint Louis, St. Louis, MO*

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TP 251 **PyViscount: Flexible Validation of FDR Estimation Methods by Search Space Partition Into Countable Sets**; Dominik Madej[1]; Henry Lam[1]; *[1]The Hong Kong University of Science and Technology, Hong Kong, Hong Kong*

TP 252 **Ion Mobility Spectrometry-Mass Spectrometry (IMS-MS) Non-Targeted Analysis Feature Screening: A method for sample classification and feature identification**; Jessie R Chappel[1]; James N. Dodds[2]; Kaylie I Kirkwood-Donelson[3]; Jonathon Fleming[1]; David M Reif[3]; Erin S. Baker[4]; *[1]North Carolina State University, Raleigh, NC; [2]University of North Carolina - Chapel Hill, Chapel Hill, NC; [3]National Institute of Environmental Health Sciences, Durham, NC; [4]University of North Carolina at Chapel Hill, Chapel Hill, NC*

TP 253 **Imputation of cancer proteomics data with a deep model that learns jointly from many datasets**; Lincoln J Harris; *University of Washington, Seattle, WA*

TP 254 **Bayesian hierachical linear models for differential protein expression analysis: dealing with data missingness**; Erik T Jansson[1]; Siri Voghera[1]; Måns Magnusson[1]; *[1]Uppsala University, Uppsala, Sweden*

TP 255 **Bias in Biomarkers? How to search multiple sample datasets in proteomics database searching software to generate accurate comparisons**; Jessica M Conforti[1]; Constantine C Breus[1]; Charli S Worth[1]; Joseph H Taube[1]; Elyssia S Gallagher[1]; *[1]Baylor University, Waco, TX*

TP 256 **Network Analysis as a Supplementary Tool for Exploratory Data Analysis in Modeling Health Outcomes based on Proteomics Data**; Monica Ghaly[1]; Zachary Dwight[1]; Susan Mockus[1]; *[1]Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Los Angeles, CA*

TP 257 **A New Approach to Matrix Library Lock Mass Correction (MLLM)**; Keith G Richardson[1]; Martin R Green[1]; Christopher J Hughes[1]; Lee A Gethings[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

TP 258 **Missingness-informed protein quantification and differential expression analysis**; Mengbo Li; *WEHI, Parkville, Australia*

TP 259 **The impact of omics normalization strategies affects grouping and differentiation of biological datasets**; Chi Yen Tseng[1, 2]; Erick S. LeBrun[1, 2]; Emilio S. Rivera[1, 2]; Tara Harvey[1, 2]; Joshua D. Breidenbach[1, 2]; Brett R. Blackwell[1, 2]; Salvator J. Palmisano[1, 2]; Grace M. Thornhill[1, 2]; Emilia A. Solomon[2]; Claire K. Sanders[3]; Marc Alvarez[2]; Kes A. Luchini[1, 2]; Abigale S Mikolitis[1, 2]; Zachary J. Sasiene[1, 2]; Ethan M. McBride[1, 2]; Austin R. Anderson[1, 2]; Lauren K. Heine[1, 2]; Jessica A. Salguero[1, 2]; Francisca E. Rodriguez[1, 2]; Phillip M. Mach[1, 2]; Trevor G. Glaros[1, 2]; *[1]Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [2]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [3]Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM*

TP 260 **JUMPsem: Enzyme Activity Inference with Structural Equation Modeling**; Dehui Kong[1]; Aijun Zhang[1]; Ling Li[1]; Zuofei Yuan[2]; Yingxue Fu[3]; Long Wu[2]; Ashutosh Mishra[2]; Anthony High[2]; Junmin Peng[2]; Xusheng Wang[1, 2]; *[1]University of Tennessee Health Science Center, Memphis, TN; [2]St.Jude Children's Research Hospital, Memphis, TN; [3]St Jude Children's Research Hospital, Memphis, TN*

TP 261 **A novel statistical similarity score using replicate electron-ionization mass spectra**; Amudhan Krishnaswamy-Usha[1]; Briana A. Capistran[1]; Edward Sisco[1]; Anthony J. Kearsley[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

TP 262 **CPred: Charge State Prediction for Modified and Unmodified Peptides in Electrospray Ionization**; Frédérique Vilenne[1]; Annelies Agten[1]; Simon Appeltans[1]; Dirk Valkenborg[1]; *[1]Hasselt University, Diepenbeek, Belgium*

TP 263 **Characterization of Peptide Ancestry Informative Markers in Lung Adenocarcinomas from Individuals of European and East Asian Ancestry**; Tamara Abulez[1]; Jeremy L Loffredo[1]; Christopher M Tarney[1]; Timothy D O'Connor[2]; Brian L Hood[1]; Glendon J Parker[3]; Kathleen M Darcy[1]; Neil T Phippen[1]; George L Maxwell[1]; Thomas P Conrads[1]; Nicholas W. Bateman[1]; *[1]Women's Health Integrated Research Center, Annandale, VA; [2]Program in Personalized and Genomic Medicine, University of Maryland School of Medicine, Baltimore, MD; [3]University of California, Davis, Davis, CA*

TP 264 **JUMP-BREAD: A User-Friendly R Shiny Tool for Streamlining Block Randomization in the Experimental Analysis and Design of Proteomics Studies**; Yingxue Fu[1]; Zuofei Yuan[2]; Long Wu[2]; Xusheng Wang[2]; Junmin Peng[2]; Anthony High[2]; *[1]St Jude Children's Research Hospital, Memphis, TN; [2]St. Jude Children's Research Hospital, Memphis, TN*

TP 265 **Assessment of false discovery rate control in tandem mass spectrometry analysis using entrapment**; Bo Wen[1]; Jack Freestone[2]; Michael J. MacCoss[1]; William S Noble[1, 3]; Uri Keich[2]; *[1]Department of Genome Sciences, University of*

Washington, Seattle, Washington; [2]Department of Statistics, University of Sydney, Sydney, Australia; [3]Paul G. Allen School of Computer Science and Engineering, University of Washington, Seattle, WA

TP 266 **A new statistical model for open search localization**; Daniel J Geiszler[1]; Nurhan Ozlu[1, 2]; *[1]Department of Molecular Biology and Genetics, Koç University, Istanbul, Turkey; [2]Koç University Research Center for Translational Medicine (KUTTAM), Koç University, Istanbul, Turkey*

TP 267 **NovoCert: Statistical validation of de novo peptide sequencing**; Shanji Zhang[1]; Seunghyuk Choi[2]; Seungjin Na[3]; Eunok Paek[1, 4]; *[1]Department of Computer Science, Hanyang University, Seoul, South Korea; [2]Baylor College of Medicine, Houston, TX; [3]Korea Basic Science Institute, Cheongju, South Korea; [4]Institute for Artificial Intelligence Research, Hanyang University, Seoul, South Korea*

TP 268 **ProtPipe2.0: A Multifunctional Data Analysis Pipeline for Proteomics, pSILAC and Peptidomics**; Ziyi Li; *NIH, Bethesda, MD*

TP 269 **Considerations Before Log-Transforming LC-MS Omics Data**; Matthew J Keller[1, 2]; Steven Tavis[1, 2]; Robert L Hettich[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Tennessee Knoxville, Knoxville, TN*

TP 270 **Assessing the Effects of Retention-Time Alignment on Protein Abundance in Proteomics Database Searching**; Constantine C Breus[1]; Jessica M Conforti[1]; Elyssia S Gallagher[1]; *[1]Baylor University, Waco, TX*

TP 271 **Beyond ion-intensity prediction: an end-to-end model for Peptide-Spectrum matching**; Maximilien Burq[1]; Jure Zbontar[1]; Juan L. Restrepo[2]; Shamil Urazbakhtin[3]; Jurgen Cox[2]; Peter Cimermancic[1]; *[1]Tesorai, San Diego, CA; [2]Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Munich, Germany; [3]Computational Systems Biochemistry Research Group, Max Planck Institute of Biochemistry, Munich, Germany*

TP 272 **Evaluating the Performance of ProteoMixture, a Proteomics-Based Cell Deconvolution Tool in Pan-Cancer Data for > 1000 Patient Tumors**; Joshua P Schaaf[1]; Tamara Abulez[1]; Pang-ning Teng[1]; Brian L Hood[1]; Kelly A Conrads[1]; Tracy J Litzi[1]; Allison L Hunt[1]; Kathleen M Darcy[1]; Neil T Phippen[1]; Thomas P Conrads[1]; Nicholas W Bateman[1]; *[1]Women's Health Integrated Research Center, Annandale, VA*

TP 273 **Scry: Scalable Data Processing for Extreme-Scale DIA Mass Spectrometry Proteomics**; Seth Just[1]; Andrew Nichols[2]; Lee Cantrell[2]; Amir Alavi[2]; Jian Wang[2]; Iman Mohtashemi[2]; Theodore Platt[2]; Serafim Batzoglou[2]; *[1]Seer, Inc, Redwood City, CA; [2]Seer, Inc., Redwood City, CA*

TP 274 **MultiplexMixer: An Enabling Utility for Rational Sample Randomization for Multiplexed, Quantitative Proteomic Workflows**; Jordan A Driscoll[1]; Tamara Abulez[1]; Kelly A Conrads[1]; Brian L Hood[1]; Kathleen M Darcy[1]; Christopher M Tarney[1]; Neil T Phippen[1]; George L Maxwell[1]; Nicholas W. Bateman[1]; Thomas P Conrads[1]; *[1]Women's Health Integrated Research Center, Annandale, VA*

TP 275 **Sin.R: A SAINT-like AP-MS protein-interaction score implemented in R**; Manor Askenazi[1]; Jackeline Ponce[2]; Beatrix Ueberheide[2]; *[1]Biomedical Hosting LLC, Arlington, MA; [2]NYU Grossman School of Medicine, New York, NY*

TP 276 **Preserving Full-Profile Information in Analysis and Compression of Imaging Mass Spectrometry Data by Sparsity-Aware Low-Rank Matrix Factorization**; Roger A.R. Moens[1]; Lukasz Migas[1]; Jacqueline Van Ardenne[2, 3]; Cody Marshall[2, 4]; David Reeves[2, 5]; Ólöf Ísberg[2, 5]; Martin Dufresne[2, 6]; Jeffrey M. Spraggins[2, 3, 4, 5, 6]; Raf Van De Plas[1, 2, 6]; *[1]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Department of Chemistry, Vanderbilt University, Nashville, TN; [4]Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN; [5]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [6]Department of Biochemistry, Vanderbilt University, Nashville, TN*

TP 277 **High Dimensional Consensus spectra for Single-Compound Forensic Drug Discrimination**; Wencheng Zhong[1]; Briana A. Capistran[2]; Amudhan Krishnaswamy Usha[2]; Edward Sisco[2]; Anthony J. Kearsley[2]; *[1]Johns Hopkins University, Baltimore, MD; [2]National Institute of Standards and Technology, Gaithersburg, MD*

TP 278 **Evaluating statistical methods and experimental designs for chemoproteomics experiments**; Sarah Szvetecz[1]; Pierre Jean Beltran[2]; Joel Federspiel[3]; Denise Field[2]; Robert J Seward[3]; Hyunsuk Suh[3]; Devon Kohler[1]; Liang Xue[2]; Olga Vitek[1]; *[1]Northeastern University, Boston, MA; [2]Pfizer, Inc, Cambridge, MA; [3]Pfizer Inc., Andover, MA*

TP 279 **MAPLE: A Pipeline for Mapping Ancestry-linked Protein Quantitative Trait Loci in Proteogenomic Data**; Satishkumar Ranganathan Ganakammal[1]; Jordan A Driscoll[1]; Tamara Abulez[1]; Christopher M Tarney[1]; Brian L Hood[1]; Kathleen M Darcy[1]; Neil T Phippen[1]; Ayman Al-Hendy[2]; George L Maxwell[1]; Thomas P Conrads[1]; Nicholas W. Bateman[1]; *[1]Women's Health Integrated Research Center, Annandale, VA; [2]University of Chicago, Chicago, IL*

TP 280 **Spectral similarity based on Siamese network model embeddings broadly outperforms standard cosine similarities on molecular networking tasks**; Gennady Voronov[1]; Daniel Ence[1]; Joe Rokicki[1]; *[1]Enveda Biosciences, Boulder, CO*

TP 281 **Run-to-run retention time alignment improves peak picking in Skyline**; Nicholas Shulman[1]; Deanna L. Plubell[1]; Brendan MacLean[1]; Michael J. MacCoss[1]; *[1]University of Washington - Genome Sciences, Seattle, WA*

TP 282 **Comparison of pQTL analysis methods on an Alzheimer's disease cohort at different sizes**; Amir Alavi[1]; Benjamin Lacar[1]; Harendra Guturu[1]; Pia Kivisakk[2]; Sudeshna Das[2]; Serafim Batzoglou[1]; Steven E. Arnold[2]; Asim Siddiqui[1]; *[1]Seer, Inc., Redwood City, CA; [2]Massachusetts General Hospital (MGH), Charlestown, MA*

TP 283 **Methods for Automated Calibration and Elemental Composition Assignment of Complex Mixtures: PyC2MC Updates**; Ryan P Rodgers[1]; Christopher L Hendrickson[2, 3]; Christopher Holder Montenegro[2, 4]; Martha L Chacon-Patino[2, 3]; Alvaro J Tello Rodriguez[2, 4]; Christopher Rüger[5]; Germain Salvato Vallverdu[3, 6]; *[1]Nat'l High Magnetic Field Lab, Tallahassee, FL; [2]National High Magnetic Field Laboratory, Tallahassee, Florida; [3]International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France; [4]Florida State University, Tallahassee, FL; [5]University of Rostock, Rostock, Germany; [6]Université de Pau et des Pays de l'Adour, Pau, France*

TP 284 **Construction of large collections of reference precursor retention times and modes across multiple tissue types**; Duong Nguyen[1, 2, 3]; Nuno Bandeira[1, 2, 3, 4]; *[1]University of California San Diego, La Jolla, CA; [2]Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; [3]Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; [4]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

TP 285 **Using First Principles to Develop Population Scale Peak Picking Software for the Genome Era: The I.A.A Suite**; Allen Hubbard[1]; Louis Connelly[1]; Rijan Dhakal[1]; Shrikaar Kambhampati[1]; Ivan Baxter[1]; *[1]Donald Danforth Plant Science Center, Saint Louis, MO*

TP 286 **Implementation of De Novo Sequencing Methods Based on a Visual Acuity Ion Classifier for Top-down, Middle-down, and Bottom-up Fragmentation Spectra**; Blake Hakkila[1]; Stephanie Sturgeon[1]; Timothy Djang[2]; Alex Gavrilenko[2]; Jhenya Gavrilenko[2]; Stelios Gkegkas[2]; Panos Iatrou[2]; Rachel Franklin[1]; Yury V. Vasilev[3]; Diana Oppenheimer[1]; Joseph Meeuswen[1]; Adrian L Guthals[1]; *[1]Agilent Technologies, Corvallis, Oregon; [2]Devicepros, Boston, USA, MA; [3]Agilent Technologies, Santa Clara, CA*

TP 287 **Accelerated Analysis of Structurally Related Components in Complex Samples**; Anne Marie Smith[1]; Alexander Lishchuk[1]; Alexander Sakharov[1]; *[1]ACD/Labs, Toronto, ON*

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TP 288 **Time-resolved characterization and analysis of pulsed ion sources by synchronized oaTOF-MS**; Franziska Schuler[1]; Joshua Rieger[1]; Maja Hammelrath[1]; Sanna Benter[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

TP 289 **Interfacing a Compact Capillary Liquid Chromatograph to a Small Footprint Triple Quadrupole Mass Spectrometer**; Serguei V. Calugaru[1]; Elisabeth P. Gates[1]; W. Raymond West[1]; Milton L. Lee[1]; Charmion I. E. Cruickshank-Quinn[2]; Wendi A. Hale[2]; David A. Jarvis[2]; *[1]Axcend, Provo, UT; [2]Agilent Technologies, Santa Clara, CA*

TP 290 **Orbitrap-based Charge Detection Mass Spectrometry using an External Data Acquisition and Processing System**; Yury Tsybin[1]; Konstantin O. Nagornov[1]; Natalia Gasilova[2]; Laure Menin[2]; Anton N. Kozhinov[1]; *[1]Spectroswiss, Lausanne, Switzerland; [2]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

TP 291 **Operating electrodynamic ion funnels in wide m/z transmission mode for simultaneous analysis of labile and non-labile analytes**; Peter Weidner[1]; Behrooz Zekavat[1]; Anabel Fandino[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 292 **Gated trapped ion mobility spectrometry coupled to Fourier transform ion cyclotron resonance mass spectrometer to characterize future green fuels**; Julien Maillard[1, 2]; Gregory Brabeck[3]; Alina Theisen[3]; Christopher Ruger[2]; Pierre Giusti[1, 2, 4]; Carlos AFONSO[2, 4]; Christopher A Wootton[3]; *[1]TotalEnergies, Harfleur, France; [2]International Joint Laboratory—iC2MC: Complex Matrices Molecular Characterization, TRTG, BP 27, 76700 Harfleur, France, Harfleur, France; [3]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; [4]University of Rouen-Normandy, Mont-Saint-Aignan, France*

TP 293 **The benefit of high power and pressure in ultra-violet photodissociation (UVPD)**; Mircea Guna[1]; Pavel Ryumin[1]; Anjali Chelur[1]; Nick Albeanu[1]; Yves Le Blanc[2]; *[1]SCIEX, Concord, ON; [2]SCIEX, Concord, On, ON*

TP 294 **Practical Quadrupole Theory: Characterization of Quadrupole Performance for Various Rod Lengths, with and without Pre-Filters**; Luke Metzler[1]; Randall E Pedder[1]; Jacob Pasko[1]; Alex Miscovich[1]; *[1]Ardara Technologies, Ardara, PA*

TP 295 **Management of a Centralized Gas Generation System in a Clinical LC-MS/MS Lab over an 11-Year Growth Period**; Brett Holmquist; *Labcorp, Calabasas Hills, CA*

TP 296 **Multivendor and Multiplatform Comparison of Linearity and Sensitivity in Mass Spectrometry Imaging**; Andrew Bowman[1]; Nari Talaty[1]; David Wagner[1]; Junhai Yang[1]; *[1]AbbVie, Inc., North Chicago, IL*

TP 297 **Different extraction mechanisms of the mass-selective axial ejection from linear quadrupole ion trap**; Fulong Deng; *Sichuan University, Chengdu, China*

TP 298 **Ion transmission characterization through a dual-field converging multipole ion guide**; Haopeng Wang[1]; Laura L Pollum[1]; Patrick M Batoon[1]; *[1]Agilent Technologies Inc., Santa Clara, CA*

TP 299 **Triple Quadrupole Mass Spectrometer Performance: Evaluation and Mitigation of Charging**; Jason D. White[1]; Michael V. Ugarov[1]; Hans Schweingruber[1]; Charles E. Maxey[1]; Neloni R. Wijeratne[1]; Claudia P.B. Martins[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 300 **Mass resolved "line-writing" and targeted area coverage for ion soft-landing**; Michael Espenship[1]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN*

TP 301 **Development of oxygen attachment dissociation (OAD)-TOF system incorporating a modified collision cell**; Yuta Miyazaki[1]; Tomoya Kudo[1]; Ryosuke Nara[1]; Hidenori Takahashi[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

TP 302 **Toward the Quantification of Ion Losses in Non-Linear Quadrupole Ion Guides in a Folded-Layout Triple Quadrupole Mass Spectrometer**; Matthias Lorenz[1]; Anna Kornilova[1]; Adrian Maclean[1]; Tak Shun Cheung[1]; Hamid Badiei[1]; *[1]PerkinElmer, Woodbridge, ON*

TP 303 **Addressing sustainability in the laboratory through the evaluation of energy consumption of a prototype benchtop LC-MS platform**; Rachel J Sanig[1]; Andrew Whatley[1]; Matthew Gibbs[1]; Lee A Gethings[1]; Gunnar Weibchen[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Eschborn, Germany*

ION MOBILITY: APPLICATIONS II
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TP 304 **Development of a Cyclic Ion Mobility Spectrometry-Mass Spectrometry (cIMS-MS)-Based Collision Cross Section Database of Permethylated Human Milk Oligosaccharides**; Sanaz C Habibi[1]; Gabe Nagy[1]; *[1]University of Utah, Salt Lake City, UT*

TP 305 **Separation of New Psychoactive Substances and Xylazine Metabolite Isomers using SLIM High-Resolution Ion Mobility-Mass Spectrometry (HRIM-MS)**; Ralph Aderorho[1]; Christopher Donald Chouinard[1]; *[1]Clemson University, Clemson, SC*

TP 306 **Trapped ion mobility spectrometry for high-throughput directed evolution screening of α-ketoglutarate dependent dioxygenases**; Robert A. Shepherd[1]; Austin R. Hopiavuori[1]; Melanie C. Jones[1]; Alex J. Tabag[1]; Conrad A. Fihn[1]; Shaun M. McKinnie[1]; Laura M Sanchez[1]; *[1]UC Santa Cruz, Santa Cruz, CA*

TP 307 **Structural Characterization of Isomeric Reaction Products using High-Resolution SLIM Ion Mobility and Computational Approaches**; Walker N Hodges[1]; Shadrack W. Lucas[1]; Ralph Aderorho[1]; Christopher Donald Chouinard[1]; *[1]Clemson University, Clemson, SC*

TP 308 **Optimization of Liquid Chromatography Trapped Ion Mobility Tandem Mass Spectrometry for Collagenase Proteomics**; Jade K. Macdonald[1]; Stephen C. Zambrzycki[1]; Richard R Drake[1]; Peggi M Angel[1]; *[1]Medical University of South Carolina, Charleston, SC*

TP 309 **Compilation of a Polysorbate CCS Database from Drift Tube and Traveling Wave Structures for Lossless Ion Manipulations Ion Mobility Measurements**; Kyle E Lira[1]; Jody C May[1]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN*

TP 310 **Ion mobility-based approaches for the separation and identification of chiral active pharmaceutical ingredients**; Valeria Guidolin[1]; Jody C. May[2]; Almary Chacon[1]; Benjamin K. Blakley[2]; Eric Dybeck[1]; John A. McLean[2]; *[1]Pfizer, Groton; [2]Vanderbilt University, Nashville, TN*

TP 311 **Evaluation of Chiral Selection Strategies with Ion Mobility-Mass Spectrometry for Differentiating Enantiomers of Drug and Drug-Like Compounds**; Benjamin K Blakley[1]; Jody C May[1]; Valeria Guidolin[2]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]Pfizer, Groton*

TP 312 **Assessing the Additivity of Mass-Distribution Based Shifts in High-Resolution Cyclic Ion Mobility Separations**; Noah D Roberts[1]; David L Williamson[1]; Gabe Nagy[1]; *[1]University of Utah, Salt Lake City, UT*

TP 313 **Ion Mobility and Collision Induced Unfolding Characterize Metal-Dependent Nucleic Acid-Protein Interactions**; Caela P Fedraw[1, 2]; Anna G Anders[1]; Nicholas J Rossiter[3]; Stephen A DeAngelo[4]; Markos Koutmos[1, 5, 6]; Costas A Lyssiotis[7, 8]; Yatrik M Shah[8, 9]; Brandon T. Ruotolo[10]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, MI; [2]Michigan Medicine Post-baccalaureate Research Education Program, University of Michigan, Ann Arbor, MI; [3]Cellular and Molecular Biology Program, University of Michigan Medical School, Ann Arbor, MI; [4]Doctoral Program in Cancer Biology, University of Michigan,* *Ann Arbor, MI; [5]Program in Biophysics, University of Michigan, Ann Arbor, MI; [6]Program in Chemical Biology, University of Michigan, Ann Arbor, MI; [7]Department of Molecular and Integrative Physiology, University of Michigan Medical School, Ann Arbor, MI; [8]Department of Internal Medicine, University of Michigan, Ann Arbor, MI; [9]University of Michigan Rogel Cancer Center, University of Michigan, Ann Arbor, MI; [10]Department of Chemistry, University of Michigan, Ann Arbor, Michigan*

TP 314 **Rapid identification and quantification of dihydroxyacetophenone positional isomers by ion mobility spectrometry time-of-flight mass spectrometry and theoretical calculations**; Chuan-Fan Ding[1]; Yinghua Yan[1]; Baichun Wang[1]; Xiaohui Huang[1]; *[1]Ningbo University, Ningbo, China*

TP 315 **High-Resolution Ion Mobility Analysis of Isomeric Bile Acids Using Structures for Lossless Ion Manipulations (SLIM) IM-MS**; Emmaleigh D Efird[1]; Makenna Hoover[1]; Terra Pettit-Bacovin[1]; Ashlee Wedge[1]; Christopher D. Chouinard[1]; *[1]Clemson University, Clemson, SC*

TP 316 **Targeted Head Group Identification for Characterizing Glycolipid Isomers Using Cyclic Ion Mobility Separations**; Cameron N Naylor[1]; Gabe Nagy[1]; *[1]University of Utah, Department of Chemistry, Salt Lake City, UT*

TP 317 **Ion mobility separation of marine natural products: Characellides from the deep sea sponge Characella pachastrelloides**; Sarah Dowd[1]; Sam Afoullouss[2]; Jennifer Netjes[2]; BIll J Baker[2]; *[1]Waters Corporation, Milford, MA; [2]University of South Florida, Tampa, FL*

TP 318 **Isolating the Effect of Moments of Inertia in High-Resolution Ion Mobility Spectrometry-Mass Spectrometry**; David L. Williamson[1]; Noah D Roberts[1]; Haisley Windsor[1]; Gabe Nagy[1]; *[1]University of Utah, Department of Chemistry, Salt Lake City, UT*

TP 319 **Method Development and Characterization of PFAS Compounds Using Structures for Lossless Ion Manipulations (SLIM) IM-MS**; Heidi Sabatini[1]; Terra Pettit-Bacovin[1]; Ralph Aderorho[1]; Christopher D. Chouinard[1]; *[1]Clemson University, Clemson, SC*

TP 320 **Structure elucidation of divarasib is mediated by alternative activation and separation strategies**; Chris M Crittenden[1]; Marcelino Varona[1]; Daniel P. Dobson[1]; José G. Napolitano[1]; *[1]Genentech Inc., South San Francisco, CA*

TP 321 **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[1]; Maria Fawaz[1]; Congliang Sun[1]; Yu Feng[1]; Athanasia Qirjollari[1]; Hubert Josien[1]; Kara M Pearson[1]; Raymond J. Gonzalez[1]; Lisa O'Callaghan[1]; Mark T. Cancilla[1]; Weixun Wang[1]; Daniel S. Spellman[1]; *[1]Merck Sharp & Dohme LLC, West Point, PA*

TP 322 **Enhanced detection and quantitation of targeted metabolites through native ion mobility-mass spectrometry and collisional ligand ejection**; Michael R Armbruster[1]; Brandon T Ruotolo[1]; *[1]University of Michigan Department of Chemistry, Ann Arbor, MI*

TP 323 **Study on the aggregation of alpha-synuclein peptides and stable oligomeric conformations using IM-MS and MD simulations**; Zhiyuan Zhu[1]; Yilei Li[1]; Michael T. Bowers[1]; *[1]UCSB, Santa Barbara, CA*

ISOTOPE LABELING AND FLUXOMICS APPLICATIONS
324-329

TP 324 **Prediction of isotopologue concentration from an AI model for unlabelled analytes: The foundation for absolute quantitation in metabolomic flux analyses**; Joshua Lauterbach[1]; Ana S.H. Costa[1]; Devesh Shah[1]; Luke S. Ferro[1]; Steven B. Hooper[1]; Jack Howland[1]; Jefferson G. Pruyne[1]; Timothy Kassis[1]; Jennifer M. Campbell[1]; *[1]Matterworks, Inc., Somerville, MA*

TP 325 **13C-metabolic flux analysis using GC-MS reveals metabolic rewiring in HL-60 neutrophil-like cells through differentiation and immune stimulation**; Takeo Taniguchi[1]; Nobuyuki Okahashi[1]; Fumio Matsuda[1]; *[1]Osaka university, Osaka, Japan*

TP 326 **An Ultra-High Throughput Cell-Based Mass Spectrometry Flux Assay as an in-situ Screening Strategy.**; Daniel P Downes[1]; Christopher M Barbieri[1]; Lisa M. Kopcho[1]; David Connors[1]; Madhu Sudhan Ravindran[2]; Wilson Z. Shou[1]; Andrew D. Wagner[1]; Brian J. Arey[1]; *[1]Bristol Myers Squibb, Princeton, NJ; [2]Syngene, Bangalore, India*

TP 327 **Application of multiple isotope pattern searches for in-depth plant metabolism determination**; Chris Brown[1]; Jeffrey R Gilbert[1]; Yelena Adelfinskaya[1]; Eva Duchoslav[2]; Yves LeBlanc[2]; *[1]Corteva Agriscience, Indianapolis, IN; [2]SCIEX, Concord, ON*

TP 328 **3D-printed stackable air-liquid interface platform with paper-based cell culture enables isotopic flux analysis of cancer volatiles via HS-SPME/GC-MS**; Hyojeong Lee[1]; Dong-kyu Lee[1]; *[1]College of Pharmacy, Chung-Ang University, Seoul, South Korea*

TP 329 **Top-Simple Light Isotope Metabolic (SLIM)-Labeling, a unique method for LC-MS-based quantification of intact proteins in complex samples.**; Jean-Michel CAMADRO[1]; Denis MESTIVIER[2]; Nicolas SENECAUT[3]; Alexia LOURENCO[4]; Victor COCHARD[1]; Marie LEY[1]; Véronique LEGROS[1]; Guillaume CHEVREUX[1]; *[1]Institut Jacques Monod CNRS, Paris, France; [2]Université Paris-Est Créteil, Créteil, France; [3]Rijksuniversiteit Groningen, Groningen, Netherlands; [4]Inovarion, Paris, France*

LC/MS: SAMPLE PREPARATION I
330-350

TP 330 **Facilitating large-scale proteomics by combining automated sample preparation with short gradient LC-MS acquisitions**; Luca Sandro Räss[1]; Sandra Schär[1]; Roland Bruderer[1]; Christopher Below[1]; Ino Karemaker[1]; Lukas Reiter[1]; *[1]BiognoSYS, Schlieren, Switzerland*

TP 331 **Simplified Detergent Facilitated End-to-End Automation of LC-MS Biopharmaceutical Peptide Mapping**; Jason L. Richardson[1]; Zhongqi Zhang[1]; *[1]Amgen, Thousand Oaks, CA*

TP 332 **Broad chemical space sample preparation and sensitive LC-MS/MS for high-throughput exposomics**; Yunyun GU[1]; Maren Kirchner[1]; Caroline Helen Johnson[2]; Benedikt Warth[1]; *[1]University of Vienna, Vienna, Austria; [2]Yale University, New Haven, CT*

TP 333 **Bringing Simplicity into Plasma Proteomics by Applying a Fast, High-Throughput and Standardized Automation Platform**; Fabian Wendt[1]; Claudia Martelli[2]; Zehan Hu[3]; Andreas Schmidt[4]; Christopher Below[5]; Roland Bruderer[5]; Katrin Hartinger[3]; Gary Kruppa[6]; Nils A. Kulak[3]; Manuel Bauer[1]; *[1]Tecan, Männedorf, Switzerland; [2]Bruker Switzerland AG, Faellanden, Switzerland; [3]PreOmics, Planegg/Martinsried, Germany; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [5]Biognosys AG, Zuerich, Switzerland; [6]Bruker S.R.O., Brno, Czech Republic*

TP 334 **Mass spectrometry-based proteomics is an orthogonal methodology to affinity-based technology**; Ann-Christine König[1]; Thomas Gronauer[1]; Andreas Schmidt[2]; Marcel Blindert[1]; Fabian Gruhn[1]; Zuzana Demianova[3]; Juliane Merl-Pham[1]; Stefanie Hauck[1]; *[1]Helmholtz Munich, Munich, Germany; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]PreOmics GmbH, München, Germany*

TP 335 **Introducing novel high-capacity and easy-to-use Empore membrane-based methods for proteome and metabolome analysis**; Gregory A Davidson[1]; Yanbao Yu[1, 2]; Guotao Lu[1]; Xiaohui Zhang[1]; *[1]CDS Analytical LLC, Oxford, PA; [2]University of Delaware, Newark, DE*

TP 336 **Characterizing Trypsin Proteoforms and Their Impact on Digestion Efficiency and Specificity**; Shailin Patel[1]; Victoria C. Cotham[1]; Shunhai Wang[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY*

TP 337 **A novel on-filter in-cell digestion (OFIC) approach enables rapid and in-depth proteome profiling of lintact cells with minimal input**; Yanbao Yu[1]; Jessica L Keffer[1]; Guotao Lu[2]; Gregory A Davidson[2]; *[1]University of Delaware, Newark, DE; [2]CDS Analytical LLC, Oxford, PA*

TP 338 **Incorporation of hydrophilic magnetic beads into proteomic workflows**; Ellen Crummy[1]; Chris Hosfield[1]; Elizabeth Caine[1]; Kristin Riching[1]; Marjeta Urh[1]; Mike Rosenblatt[1]; *[1]Promega Corporation, Madison, Wisconsin*

TP 339 **Proteomics analysis of limited number of cells by a rapid and efficient workflow using adaptive focused acoustic technology**; Anu Jain[1]; M Cristine C. Charlesworth[2]; Sameer Vasantgadkar[3]; Debadeep Bhattacharyya[3]; Akhilesh Pandey[2]; *[1]Mayo Clinic, Rochester, MN; [2]Mayo clinic, Rochester, MN; [3]Covaris, LLC, Woburn, MA*

TP 340 **Streamlined Proteomic Sample Preparation: On-Column Protein Digestion coupled to Automated Peptide Desalting**; Heather Eastwood[1]; Fabian Wendt[2]; Qi Huang[1]; John D Laycock[1]; *[1]Tecan, Baldwin Park, CA; [2]TECAN Group, Männedorf, Switzerland*

TP 341 **Development of an LCMS method for polyamine analysis using carbonylated derivatives**; Megan R Gendjar[1]; Christine Isaguirre[1]; Ryan D Sheldon[1]; *[1]Van Andel Research Institute, Grand Rapids, MI*

TP 342 **Evaluating Sample Preparation methods in a Core facility environment for samples with low amounts of protein**; Gabriela Grigorean[1]; Lauren Yoon Dixon[1]; Brett S. Phinney[1]; *[1]University of California - Davis, Davis, CA*

TP 343 **Benchmarking magnetic Streptavidin beads for high-throughput enrichment of biotinylated proteins**; Vineet Vaibhav[1, 2]; Toby Dite[1, 2]; Jumana Yousef[1, 2]; Ryan S Cross[1, 3]; Alexander J Davenport[1, 3]; Misty R Jenkins[1, 3]; Laura F Dagley[1, 2]; *[1]WEHI, Parkville, Australia; [2]Department of Medical biology, University of Melbourne, Melbourne, Australia; [3]Immunology Division, The Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia*

TP 344 **Method development for the simultaneous analysis of drugs of abuse in fish tissue**; DIANA M CARDENAS SORACA[1]; Paola A. Ortiz-Suarez[2]; Sandra Salic[2]; Rashne Vakharia[2]; Leslie M. Bragg[2]; Mark R. Servos[2]; *[1]UNIVERSITY OF WATERLOO, Waterloo, ON; [2]University of Waterloo, Waterloo, ON*

TP 345 **Solid Phase Extraction Of Fentanyl Analogs And Xylazine In Urine Using HPSCX Columns On The Resolvex® i300/A200 Instruments**; Heather Eastwood[1]; Steven Alo[1]; Qi Huang[1]; Karsten Liegmann[1]; John D Laycock[1]; *[1]Tecan, Baldwin Park, CA*

TP 346 **Rapid, Semi-automated Enzyme Profiling**; Jolene K Diedrich[1, 2]; Antonio F. M. Pinto[2]; Casimir Bamberger[1]; John R. Yates III[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Salk Institute for Biological Studies, La Jolla, CA*

TP 347 **High throughput proteomics analyses of Immunoglobulin bound and circulating free proteins in human plasma**; Huiling Liu[1]; Hiroyuki Katayama[1]; Yining Cai[1]; Johannes Francois Fahrmann[1]; Jody Vykoukal[1]; Matthew Willetts; Diego Assis[2]; Elizabeth Gordon[2]; Samir Hanash[1]; *[1]Department of Clinical Cancer Prevention, The University of Texas MD Anderson Cancer Center, Houston, TX; [2]Bruker Scientific LLC, Billerica, MA*

TP 348 **Navigating the inherent challenges with dilute and shoot: an investigation using protein depletion plates**; Lauren E Seveney; *Dominion Diagnostics, LLC, North Kingstown, RI*

TP 349 **Benchmarking a low-cost automated sample preparation platform for highly multiplexed blood plasma proteomics**; Eric F. Zaniewski[1, 2]; Benedikt C. Clemens[1, 2]; Robert Morris[1, 2]; Johannes Kreuzer[1, 2]; Soroush Hajizadeh[1, 2]; Marc S. Weinberg[1, 2]; Mahesh Chandra Kodali[1, 2]; Pia Kivisakk[1, 2]; Steven E. Arnold[1, 2]; Wilhelm Haas[1, 2]; *[1]Massachusetts General Hospital (MGH), Charlestown, MA; [2]Harvard Medical School, Boston, MA*

TP 350 **Optimized instrument configuration for the Orbitrap Astral mass spectrometer in data-dependent acquisition (DDA) and data-independent acquisition (DIA) modes**; Ivo A Hendriks[1]; Sara C. Buch-Larsen[1]; Martin Rykær[1]; Michael L Nielsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, København, Denmark*

LIPIDS: GENERAL
351-383

TP 351 **Bi-Modal Fluorescence-Mass Spectrometry for Lipid Characterization**; Dallas Freitas[1]; Gopal Reddy[1]; Xin Yan[1]; *[1]Texas A&M, College Station, TX*

TP 352 **Building a Multidimensional Oxylipin Library Containing Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry Information**; Amie M. Solosky[1]; Olivier Salamin[2]; Jack P. Ryan[1]; James N. Dodds[1]; Craig E. Wheelock[2, 3]; Erin S. Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Karolinska Institutet, Stockholm, Sweden; [3]Karolinska University Hospital, Stockholm, Sweden*

TP 353 **Comparing Storage Conditions for the Analysis of Extracted Lipids from Latent Fingerprints: Liquid Extracts vs Frozen Foils**; Aleesa E Chua[1]; Eden P. Go[1]; Heather Desaire[1]; *[1]University of Kansas, Lawrence, KS*

TP 354 **Kinetic isotopic tracing unravels the de novo synthesis and metabolism of phospholipid isomers at C=C location level**; Zhuoning Xie[1]; Zheng Ouyang[1]; Xiaoxiao Ma[1]; *[1]Tsinghua University, Beijing, China*

TP 355 **Lipid labeling method to identify alternative carbon sources during glucose starvation**; Rebekah L Mokry[1, 2]; John G Purdy[1, 2, 3]; *[1]BIO5 Institute, University of Arizona, Tucson, AZ; [2]Department of Immunobiology, University of Arizona, Tucson, AZ; [3]Cancer Biology Interdisciplinary Program, University of Arizona, Tucson, AZ*

TP 356 **Formation of iron adduct ions of some Polyunsaturated fatty acids under ESI conditions: Potential suppression of overall LC-MS sensitivity**; Josef Ruzicka[1]; France Landry[1]; Petia Shipkova[1]; *[1]Bristol Myers Squibb, Lawrenceville, NJ*

TP 357 **Analysis of Enterococcus faecalis Glycerophospholipids and Fatty Acid Incorporation by Ion Mobility-Mass Spectrometry and Paternò-Büchi C=C Analysis**; Rebekah L Phelan[1]; Hannah M Hynds[1]; Kelly M Hines[1]; *[1]University of Georgia, Athens, GA*

TP 358 **Stability Study of mRNA- Lipid Nanoparticles under Different Formulation and Storage Conditions**; David Wong[1]; Suresh Babu Cv[2]; Ravindra Gudihal[2]; Li Zhang[3]; Yi Yan Yang[3]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies Singapore (sales) Pte Ltd, Singapore, Singapore; [3]Bioprocessing Technology Institute, Agency for Science, Technology and Research, Singapore, Singapore*

TP 359 **Analysis of Lipid Nanoparticle Components by MALDI Trapped Ion Mobility Spectrometry**; Sergei Dikler; *Bruker Scientific, LLC, Billerica, MA*

TP 360 **Analysis of Tissue Lipid Incorporation by Staphylococcus aureus**; David T Brewer[1]; Kelly M. Hines[1]; *[1]University of Georgia, Athens, GA*

TP 361 **Fast Lipid Analysis of Lipid A Coupled with Tandem Mass Spectrometry**; Katelynn S. Zuercher[1]; Erin H. Seeley[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

TP 362 **Gordonia amarae and Mycobacterium tuberculosis mycolic acid isomers revealed by cyclic ion mobility (cIM)-mass spectrometry (MS).**; Hector De Las Heras Prieto[1]; Rachel Schwartz-Narbonne[1]; Laura Cole[1]; Martin Palmer[2]; Sarah Forbes[1]; *[1]Sheffield Hallam University, Sheffield, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom*

TP 363 **Characterization of Complex Cardiolipins by Liquid Chromatography with Hybrid CID and UVPD**; Olivia E Dioli[1]; Melanie J Campbell[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, Texas*

TP 364 **Phosphatidylethanol Signatures in Blood May Help Determine Patterns of Alcohol Consumption**; Sangeeta Pandey[1]; Harmeet Kaur Chohan[1]; Peter L. Anderson[2]; Kristina M. Brooks[2]; R. Graham Cooks[1]; *[1]Purdue University, Department of Chemistry, West Lafayette, IN; [2]University of Colorado, Anschutz Medical Campus, Department of Pharmaceutical Sciences, Aurora, CO*

TP 365 **Minimizing Lipid Fragmentation Utilizing HPLC-Ultrasonic Nebulization-Corona Discharge Ionization Mass Spectrometry (HPLC-USN-CD-MS)**; Qian Ma[1]; Theresa Evans-Nguyen[1]; *[1]University of South Florida, Tampa, FL*

TP 366 **Untargeted LC-MS characterization of human breast tumor cell lines reveals subtype-specific differences in the lipidome**; William D. Gwynne[1]; Nicholas S. Ly[1]; Jeremy K. Chan[1]; Brandon Y. Lieng[1]; Olivia Taverniti[1]; Andrew T. Quaile[1]; J. Rafael Montenegro-Burke[1]; *[1]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON*

TP 367 **Lipidomics: How much do materials matter?**; Whitney L Stutts; *North Carolina State University, Raleigh, NC*

TP 368 **Unlocking E. Coli's lipidomes: delving into the dynamic composition of different strains**; Amy K Wycislik[1]; Adriana Zardini Buzatto[1, 2]; *[1]University of Calgary, Calgary, AB; [2]Calgary Metabolomics Research Facility, Calgary, AB*

TP 369 **Optimization of a micro-LC-MS/MS method for untargeted Lipidomics**; Fernanda Sousa Monteiro[1]; Liang Li[1, 2]; *[1]University of Alberta, Edmonton, AB; [2]The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta*

TP 370 **Lipidomics reveals altered hepatic lipid metabolism in response to acetaminophen overdose**; Ahsan Hameed[1, 2]; Colin D. Kay[3]; Mario G. Ferruzzi[3]; Andrew J Morris[3, 4, 5]; Mitchell McGill[6]; *[1]Arkansas Children's Nutrition Center, Little Rock, AR; [2]Department of Pediatrics, University of Arkansas for Medical Sciences, Little Rock, AR; [3]Arkansas Children's Nutrition Center, University of Arkansas for Medical Sciences, Little Rock, AR; [4]Department of Pharmacology and Toxicology, University of Arkansas for Medical Sciences, Little Rock, AR; [5]Central Arkansas Veterans Affairs Healthcare System, Little Rock, AR; [6]Department of Environmental Health Sciences, Fay W. Boozman College of Public Health, University of Arkansas for Medical Sciences, Little Rock, AR*

TP 371 **Lipids as Indicators of Successful Fecal Microbiota Transplantations**; Guozhi Zhang[1]; Arthur S. McMillan[2]; Jessie R. Chapel[2]; Casey M. Theriot[2]; Erin S. Baker[1]; *[1]UNC-Chapel Hill, Chapel Hill, NC; [2]North Carolina State University, Raleigh, NC*

TP 372 **Lipidomics of NASH human liver organoids align with liver biopsies of NASH patients**; Nate F Schmidt[1]; Ekta Minocha[1]; Ashwani Gupta[1]; Jason Wertheim[1]; Richard Green[2]; John G Purdy[1]; *[1]BIO5 Institute, University of Arizona, Tucson, AZ; [2]Northwestern University Feinberg School of Medicine, Chicago, IL*

TP 373 **Investigating the Role of Circulating small extracellular vesicles Lipids in Prostate Cancer**; Marco Ghirimoldi[1]; Marco Falasca[2]; Marcello Manfredi[3]; Elettra Barberis[4]; *[1]University of Piemonte Orientale, Novara, Italy; [2]Università di Parma, Parma, Italy; [3]DIMET, Novara, Italy; [4]DISIT, Alessandria, Italy*

TP 374 **Probing the Environmental Fortitude of mRNA Lipid Nanoparticles: A TIMS-TOF Insights into Stress-Induced Degradation**; Michael Girgis[1]; Beixi Wang[2]; Xuejun Peng[2]; Hooda Said[1]; Suman Alishetty[1]; Manuel Carrasco[1]; Dillon O'neill[1]; Nabilah Baby[1]; Gregory Petruncio[1]; Mohamad-Gabriel Alameh[3]; Caroline Hoemann[1]; Matthew Albano[4]; Erica Marie Forsberg[2]; Mikell Paige[1]; *[1]George Mason University, Manassas, VA; [2]Bruker Scientific LLC, San Jose, CA; [3]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; [4]Bruker Scientific, LLC, Billerica, MA*

TP 375 **One-Step Lipid Mass Tags for Probing Unsaturated Lipid Isomers and Accurate Relative Quantification**; Gopal Reddy Ramidi[1]; Tingyuan Yang[1]; Xin Yan[1]; *[1]Texas A&M University, College Station, TX*

TP 376 **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[1]; Nyasha Munjoma[1]; Robert S Plumb[2]; Jason Hill[2]; Nick Tomczyk[1]; Lee A Gethings[1]; Richard Lock[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA*

TP 377 **Complex Lipid Mixture Analysis using Homemade SPE-ESI-MS**; Octavion Spears[1]; Alex Grooms[2]; Benjamin Burris[2]; Abraham K. Badu-Tawiah[2]; *[1]The Ohio State University, Columbus, OH; [2]Ohio State University, Columbus, OH*

TP 378 **Impact of Contaminants from Plasticware Used in Sample Preparation on Human Serum Lipidome Analysis**; Carlos R. Canez[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*

TP 379 **nano-lipidomics employing silica based monolithic columns**; Matthias Schittmayer-Schantl[1]; Goran Mitulovic[2]; Michael Krawitzky[2]; Gary Kruppa[3]; Ruth Birner-Gruenberger[1]; *[1]TU Wien, Vienna, Austria; [2]Bruker Switzerland AG, Faellanden, Switzerland; [3]Bruker S.R.O., Brno, Czech Republic*

TP 380 **Assessing changes in sebum lipids according to anatomical collection region and biological sex**; Madeline Isom[1]; Eden P. Go[1]; Heather Desaire[1]; *[1]The University of Kansas, Lawrence, KS*

TP 381 **Monitoring the Exchange of Cholesterol Between Nanodiscs by APCI**; Annika Silverberg[1]; Michael Marty[1]; *[1]University of Arizona, Tucson, AZ*

TP 382 **Using data-dependent and independent hybrid acquisitions for fast liquid chromatography-based untargeted lipidomics**; Kanako Tokiyoshi[1]; Yuki Matsuzawa[1]; Mikiko Takahashi[2]; Hiroaki Takeda[1, 3]; Kozo Nishida[1]; Mayu Hasegawa[4]; Junki Miyamoto[4]; Hiroshi Tsugawa[1, 2, 3, 5, 6]; *[1]Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology, Koganei-shi, Japan; [2]RIKEN Center for Sustainable Resource Science, Yokohama, Japan; [3]RIKEN Center for Brain Science, Wako, Japan; [4]Department of Applied Biological Science, Tokyo University of Agriculture and Technology, Fuchu, Japan; [5]RIKEN Center for Integrative Medical Sciences, Yokohama, Japan; [6]Molecular and Cellular Epigenetics Laboratory, Graduate School of Medical Life Science, Yokohama City University, Yokohama, Japan*

TP 383 **Resolving Method Development Challenges in the Assay Validation of PEG-Lipid Quantitation**; Melissa Roberts[1]; Ryan Lo[1]; Ling Morgan[1]; *[1]Moderna, Cambridge, MA*

LIPIDS: ID AND STRUCTURAL ANALYSIS II
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TP 384 **Localization of lipid C=C bond positions using nitroarenes via photoirradiation and mass spectrometry**; Xi Chen[1]; Gopal Reddy Ramidi[1]; Annesha Sengupta[1]; Luchen Wuyang[1]; Aidan Slagter[1]; Nitya Shree[2]; Mahua Choudhury[2]; Xin Yan[1]; *[1]Department of Chemistry, Texas A&M University, College Station, TX; [2]Department of Pharmaceutical Sciences, Texas A&M University, College Station, TX*

TP 385 **Chemical Conjugation Method for Enhanced Diacylglycerol Multiple Reaction Monitoring Profiling**; Harshit Arora[1]; Pooja Saklani[2]; Guang Yang[2]; Caitlin Randolph[3]; Gaurav Chopra[2, 4, 5, 6, 7, 8]; *[1]PURDUE UNIVERSITY, West Lafayette, IN; [2]Purdue University, Department of Chemistry, West Lafayette, IN; [3]Purdue University Department of Chemistry, West Lafayette, IN; [4]Purdue Institute for Drug Discovery, West Lafayette, IN; [5]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; [6]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; [7]Purdue Institute for Integrative Neuroscience, West Lafayette, IN; [8]Purdue University, Department of Computer Science, West Lafayette, IN*

TP 386 **Analysis of novel Caenorhabditis elegans-specific phosphorylated sphingolipids using LC-TIMS-MS/MS and MassQL**; Michael Witting[1, 2]; Liesa Salzer[3]; Sven Myer[4]; Aiko Barsch[4]; Russell Waugh[5]; *[1]Metabolomics and Proteomics Core, Helmholtz Zentrum München German Research Center for Environmental Health, Neuherberg, Germany; [2]Chair of Analytical Food Chemistry, TUM School of Life Sciences, Technical University of Munich, Freising-*

Weihenstephan, Germany; [3]Research Unit Analytical BioGeoChemistry, Helmholtz Zentrum München German Research Center for Environmental Health, Neuherberg, Germany; [4]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; [5]Bruker Scientific LLC, Denver, CO

TP 387 **Photochemical Tissue Pre-processing for Matrix-Assisted Laser Desorption Ionization Imaging of Lipids**; Taylar Bell[1]; Kadeem O Hayes[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

TP 388 **Multidimensional Characterization of Oxidized Lipids Using HILIC - Ion Mobility - Mass Spectrometry**; Noelle Reimers[1]; Libin Xu[2]; *[1]University of Washingon, Seattle, WA; [2]University of Washington, Seattle, WA*

TP 389 **Novel Ion Fragmentation for Detailed Lipid Structual Analysis via Atomic Hydrogen/Oxygen Irradiation (HAD/OAD)**; Hidenori Takahashi[1]; Yohei Arao[1]; Kaoru Nakagawa[1]; Yuta Miyazaki[1]; Takanari Hattori[1]; Natsuyo Asano[1]; *[1]Shimadzu, Kyoto, Japan*

TP 390 **Charge switching isomeric and isobaric lipid cations for chemical separation with subsequent carbon-carbon double bond localization**; Kimberly C. Fabijanczuk[1]; Boukar K. S. Faye[1]; Catilin E. Randolph[1]; Scott A. McLuckey[1]; *[1]Purdue University, Department of Chemistry, West Lafayette, IN*

TP 391 **Charge Switching OzESI-MRM Strategy for Isomer-Specific Fatty Acid Profiling of Lipid Droplets with Relation to Alzheimer's Disease and Aging**; Caitlin Randolph[1]; Palak Manchanda[1]; Sanjay Iyer[1]; Shane Tichy[2]; Gaurav Chopra[1, 3, 4, 5, 6, 7]; *[1]Purdue University, Department of Chemistry, West Lafayette, IN; [2]Agilent Technologies, Santa Clara, CA; [3]Purdue Institute for Integrative Neuroscience, West Lafayette, IN; [4]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; [5]Purdue University, Department of Computer Science, West Lafayette, IN; [6]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; [7]Purdue Institute for Drug Discovery, West Lafayette, IN*

TP 392 **A Novel Structure-Driven Predict-to-Hit Strategy for PC Double Bonds Positional Isomers Identification Based on Negative LC-MRMAnalysis**; Xin Zheng[1]; Cai Tie[2]; Xinge Cui[1]; *[1]Peking Union Medical College Hospital, Beijing, China; [2]China University of Mining and Technology-Beijing, Beijing, China*

TP 393 **High Resolution Ion Mobility Incorporating Traveling Wave Structures for Lossless Ion Manipulation Unveils Hidden Lipid Features within Total Lipid Fractions**; Allison R Reardon[1]; Katrina L Leaptrot[1]; Jody C May[1]; John A McLean[1]; *[1]Vanderbilt University, Nashville, TN*

TP 394 **Spatial mapping of phosphatidylcholine sn-position isomers using CID of divalent metal complexes in imaging mass spectrometry**; Tingting Yan[1]; Zunaira Naeem[1]; Boone M. Prentice[1]; *[1]The University of Florida, Gainesville, FL*

TP 395 **Lipid A double bond position determination using ozone and laser-induced dissociation**; ABANOUB MIKHAEL[1, 2]; HELENA PETROSOVA[1, 2]; DEREK SMITH[2]; ROBERT K ERNST[3]; DAVID R GOODLETT[1, 2]; *[1]University of Victoria, Victoria, BC; [2]University of Victoria Genome BC Proteomic Centre, Victoria, British Columbia; [3]University of Maryland, Baltimore, Baltimore, MD*

TP 396 **Resolving the Geometry and Location of Lipid Unsaturation by Radical-Induced Isomerization and RPLC-MS/MS Coupled with Online Paternò-Büchi Reaction**; Hengxue Shi[1]; Yu Xia[1]; *[1]Tsinghua University, Beijing, China*

TP 397 **Deep profiling of phosphoinositide phosphates from cells and organelles**; Zidan Wang[1]; Xue Jin[1]; Hanlin Ren[2]; Shuaiting Yan[1]; Hang Yin[1]; Yu Xia[1]; *[1]Tsinghua University, Beijing, China; [2]The University of Texas at Austin, Austin, TX*

TP 398 **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[1]; Mays Al-Dulaymi[2]; Zhichang Yang[3]; Sahana Mollah[4]; Jonathan Le Huray[2]; Roxana McCloskey[1]; *[1]Sciex, Framingham, MA; [2]Acuitas Therapeutics Inc., Vancouver, BC; [3]Genentech, Inc., South San Francisco, CA; [4]SCIEX, Redwood City, CA*

TP 399 **Deep profiling of gut bacteria lipidome via data-dependent acquisition and radical-directed dissociation-tandem mass spectrometry**; Ruijun Jian[1]; Xiaoqi Zhu[2]; Hailiang Liu[2]; Yu Xia[1]; *[1]Tsinghua University, Beijing, China; [2]State Key Laboratory of Cardiology and Medical Innovation Center, Shanghai East Hospital, School of Medicine, Tongji University, Shanghai, China*

TP 400 **Characterizing Lipid Isomers Using Superior Ion Mobility Separations and Ultrafast Ozone-Induced Dissociation of Multiply Charged Transition Metal Complexes**; Alexandre A Shvartsburg[1]; Hayden A Thurman[1]; Pawel Sadowski[2]; Berwyck LJ Poad[2]; Stephen J Blanksby[2]; *[1]Wichita State University, Wichita, KS; [2]Queensland University of Technology, Brisbane, Australia*

TP 401 **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[1]; Paolo Redegalli[2]; Alan Barnes[1]; Olga Deda[3]; Thomas Meikopoulos[3]; Christina Virgiliou[3]; Helen Gika[3]; Neil J Loftus[1]; *[1]Shimadzu Corporation, Manchester, United Kingdom; [2]Shimadzu Italia S.r.l., Milano, Italy; [3]BIOMIC_AUTh, CIRI, Aristotle University of Thessaloniki, Thessaloniki, Greece*

TP 402 **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[1]; Stefan König[2]; Gérard Hopfgartner[1]; *[1]University of Geneva, Geneva, Switzerland; [2]University of Bern, Bern, Switzerland*

TP 403 **Empirically determined adduct ratios and in-source fragments enhance lipid species identification**; Nicholas S Ly[1]; Jeremy K Chan[1]; William D Gwynne[1]; Brandon Y Lieng[1]; Andrew T Quaile[1]; Cunjie Zhang[1]; J. Rafael Montenegro-Burke[1]; *[1]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON*

METABOLOMICS: CLINICAL APPLICATIONS
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TP 404 **Neonatal Metabolomics: The Untold Stories in Infant's Blood**; Carter Asef[1]; Samuel G. Moore[1]; C. Austin Pickens[2]; Carlos A. Saavedra-Matiz[3]; Joseph J. Orsini[3]; Konstantinos Petritis[2]; David A. Gaul[1]; Facundo M. Fernandez[1, 4]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Altanta, GA; [2]Division of Laboratory Sciences, National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, GA; [3]Newborn Screening Program, Wadsworth Center, New York State Department of Health, Albany, NY; [4]Petit Institute of Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA*

TP 405 **Identification of urine metabolic biomarkers for diagnosing membranous nephropathy and its subtype**; Yufei Li[1]; Ji Hye Kim[2]; Jihyun Kang[1, 3]; Seung Seok Han[4]; Joo-Youn Cho[1, 5]; *[1]Department of Clinical Pharmacology and Therapeutics, Seoul National University College of Medicine and Hospital, Seoul, South Korea; [2]Department of Internal Medicine, Chungbuk National University Hospital, Seoul, South Korea; [3]Kidney Research Institute, Seoul National University Medical Research Center, Seoul, South Korea; [4]Department of Internal Medicine, Seoul National University College of Medicine, Seoul, South Korea; [5]Department of Biomedical Sciences, Seoul National University College of Medicine, Seoul, South Korea*

TP 406 **Metabolomic Profiling Reveals Alterations in Arginine Biosynthesis Induced by β-Lapachone Derivative**; YEONSEO JANG[1]; Jihyun Kang[1, 2]; Yufei Li[1]; Eunsol Yang[1, 3]; SeungHwan Lee[1]; Joo-Youn Cho[1, 4]; *[1]Department of Clinical Pharmacology and Therapeutics, Seoul National University College of Medicine and Hospital, Seoul, South*

Korea; [2]Kidney Research Institute, Seoul National University Medical Research Center, Seoul, South Korea; [3]Department of Bioengineering and Therapeutic Sciences, University of California, San Fransisco, San Fransisco, CA; [4]Department of Biomedical Sciences, Seoul National University College of Medicine, Seoul, South Korea

TP 407 **Screening of organic acids for nutritional and metabolic profiling from dried urine spots using Gas Chromatograph Mass Spectrometer**; Aseem Rajan Wagle[1]; Prashant Hase[1]; Bhaumik Trivedi[1]; Sanket Chiplunkar[1]; Durvesh Sawant[1]; Rahul Dwivedi[1]; Hemant Kesarkar[1]; Mohit Sharma[1]; Satyendra Singh[1]; Pratap Rasam[1]; Jitendra Kelkar[1]; *[1]Shimadzu Analytical India Pvt. Ltd., Mumbai, India*

TP 408 **Untargeted metabolomic and lipidomic analyses reveal renal complications in COVID-19: molecular insights from a pilot study**; Patrick Ferreira[1]; Lucia Andrade[2]; Alessandra Sussulini[1, 3]; *[1]Laboratory of Bioanalytics and Integreted Omics (LaBIOmics), University of Campinas (UNICAMP), Campinas, Brazil; [2]Basic Research Laboratory in Renal Diseases, Faculty of Medicine, University of São Paulo (USP), São Paulo, Brazil; [3]National Institute of Science and Technology of Bioanalytics (INCTBio), University of Campinas (UNICAMP), Campinas, Brazil*

TP 409 **Diagnostic Biomarker Discovery Platform for Malignant Pancreatic Cysts by LC-HR-MS with Targeted and Untargeted Data Analysis**; Li Zhang[1]; Hong Sun Kim[2]; Harrison Wong[3]; Costas A Lyssiotis[3]; Jiaqi Shi[2]; *[1]University of Michigan, Ann Arbor, MI; [2]Department of Pathology, University of Michigan, Ann Arbor, Michigan 48109, United States, Ann Arbor, Michigan; [3]University of Michigan, Medical School, Ann Arbor, Michigan*

TP 410 **Establishing a high throughput LC-MS based metabolomics study for the deep phenotyping of plasma sample from cohorts investigating heart failure**; Fabian Schmitt[1]; Thierry Schmidlin[1]; *[1]Institute of Immunology, University Medical Center of the Johannes-Gutenberg University, Mainz, Germany*

TP 411 **Antidepressant screening via Andrew+ sample preparation automation and LC-MS/MS to access microbiota and drug interactions**; Charlotte Hemmila[1]; Christopher Basting[2]; Sophia Lebakken[2]; Melisa Bailey[2]; Erik Swanson[2]; Courtney Broedlow[2]; Tim Griffin[1]; Emily M Cherenack[3]; Nichole R Klatt[2]; Candace Guerrero[1, 2]; *[1]University of Minnesota, Center for Metabolomics and Proteomics, Minneapolis, MN; [2]University of Minnesota, Department of Surgery, Division of Surgical Outcomes and Precision Medicine Research, Minneapolis, MN; [3]University of Miami, Miller School of Medicine, Department of Psychiatry and Behavioral Sciences, Miami, FL*

TP 412 **Supraphysiological vitamin C dosing in cancer patients and healthy controls reveals products of oxidative stress in the catabolism of heme**; Philenroza Thavrin[1, 2, 3]; Jaewoo Choi[2]; Ping Chen[4]; Paige Jamieson[2, 5]; Qi Chen[4]; Jeanne Drisko[6]; Jan F. Stevens[2, 3]; *[1]College of Science, Oregon State University, Corvallis, OR; [2]Linus Pauling Institute, Oregon State University, Corvallis, OR; [3]College of Pharmacy, Oregon State University, Corvallis, OR; [4]Department of Pharmacology, Toxicology & Therapeutics, University of Kansas Medical Center, Kansas City, KS; [5]College of Health, Oregon State University, Corvallis, OR; [6]Department of Internal Medicine, Integrative Medicine Research, University of Kansas Medical Center, Kansas City, KS*

TP 413 **Investigating the post-prandial metabolome under different food intake conditions with semi-targeted LC-MS/MS**; Jiangwen Dong[1, 2]; Yi Ning Yong[3]; Leroy Pakkiri[1, 2]; Gloria Leung[4]; Christiani Jeyakumar Henry[3, 5]; Sumanto Haldar[3]; Maxine Bonham[4]; Chester Lee Drum[1, 2]; *[1]Cardiovascular Research Institute (CVRI), National University Health System (NUHS), Singapore, Singapore; [2]Department of Medicine, Yong Loo Lin School of Medicine, National University of Singapore (NUS), Singapore, Singapore; [3]Clinical Nutrition Research Centre (CNRC), Singapore Institute of Food and Biotechnology Innovation (SIFBI), Agency for Science, Technology and Research (A*STAR), Singapore, Singapore; [4]Department of Nutrition, Dietetics and Food, Monash University, Melbourne, Australia; [5]Department of Biochemistry, National University of Singapore (NUS), Singapore, Singapore*

TP 414 **Olaris Global Panel (OGP): A highly accurate and reproducible triple quadrupole mass spectrometry-based metabolomics method for clinical biomarker discovery**; Masoumeh Dorrani[1]; Jifang Zhao[1]; Nihel Bekhti[1]; Alessia Trimigno[1]; Elizabeth O'Day[1]; Jurre J. Kamphorst[1]; *[1]Olaris, inc, Framingham, MA*

TP 415 **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[1]; Kazuki Ikeda[1]; Kosuke Hata[1]; Takeshi Bamba[1]; Yoshihiro Izumi[1]; *[1]Medical Institute of Bioregulation, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka-shi, Japan*

TP 416 **Deep Metabolic Phenotyping of Newborn Cord Blood Reveals Maternal Fetal Interactions and Disease Risk**; Samuel M Lancaster[1]; Samson Mataraso[1]; Jonathan Reiss[1]; Kévin Contrepois[2]; Casandra Trowbridge[1]; Basil Michael[1]; Ian Simms[1]; Michelle Gibson[1]; Max Clary[1]; Lettie McGuire[1]; Frank Wong[1]; Ethan Canfield[1]; Daniel Cotter[1]; Tao Wang[1]; Yan Yang[1]; Ramesh Nair[1]; Ylayaly Katherine Bianco[1]; Jon Bernstein[1]; David Stevenson[1]; Tina Cowan[1]; Nima Aghaeepour[1]; Maya Kasowski[1]; Karl Sylvester[1]; Michael Snyder[1]; *[1]Stanford University, Stanford, CA; [2]AstraZeneca, South San Francisco, CA*

TP 417 **Plasma Metabolomics Evaluation Reveals SARS-CoV-2 Infection Disrupts Tryptophan and Energy Pathways with Correlations to Inflammation and Renal Status**; Jinchun Sun[1]; Megan Peters[1]; Li-Rong Yu[1]; Vikrant Vijay[1]; Heather Smallwood[2]; Richard Beger[1]; *[1]NCTR / USFDA, Jefferson, AR; [2]University of Tennessee Health Science Center, Memphis, TN*

TP 418 **Application of Dried Blood Spot Microsampling for High-Throughput Four-Dimensional Trapped Ion Mobility Spectrometry Lipidomics**; Jayden Lee Roberts[1, 2]; Luke Whiley[1, 2, 3]; Nicola Gray[1, 2]; Melvin Gay[4]; Xuejun Peng[5]; Elaine Holmes[1, 2, 6]; Julien Wist[1, 2, 7]; Jeremy K Nicholson[1, 2, 8, 9]; Nathan G Lawler[1, 2]; *[1]Australian National Phenome Centre, Health Futures Institute, Harry Perkins Institute, Murdoch University, Murdoch, Australia; [2]Centre for Computational and Systems Medicine, Health Futures Institute, Harry Perkins Institute, Murdoch University, Murdoch, Australia; [3]Perron Institute for Neurological and Translational Sciences, Nedlands, Australia; [4]Bruker Pty Ltd, Preston, Australia; [5]Bruker Daltonics Inc., San Jose, CA; [6]Department of Metabolism Digestion and Reproduction, Imperial College London, London, United Kingdom; [7]Chemistry Department, Universidad del Valle, Melendez, Colombia; [8]Department of Cardiology, Fiona Stanley Hospital, Medical School, University of Western Australia, Murdoch, Australia; [9]Institute of Global Health Innovation, Faculty of Medicine, Imperial College, South Kensington, United Kingdom*

TP 419 **Metabolic profiling of amniotic fluid by differential isotope dansylation labeling LC-MS for application in trisomy 21 fetuses**; Yi-Ting Chen[1]; Ya-Ju Hsieh[1]; Yao-Lung Chang[2]; Liang Li[3]; Jau-Song Yu[1]; *[1]Chang Gung University, Taoyuan, Taiwan; [2]LinKou Chang Gung Memorial Hospital, Taoyuan, Taiwan; [3]University of Alberta, Edmonton, AB*

TP 420 **Exploring effects of particulate matter exposure on pregnant women via urinary metabolic profiling**; Minki Shim[1]; Sunwha Park[2]; Young Ju Kim[2]; Dong-Kyu Lee[1]; *[1]College of Pharmacy, Chung-Ang University, Seoul, South Korea; [2]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 421 **2-Homoectoine: A New Ectoine Derivative from Phyto- and Bacterioplankton Involved in Osmoadaptation**; Muhaiminatul Azizah[1]; Georg Pohnert[1, 2]; *[1]Friedrich Schiller University Jena, Jena, Germany; [2]Max Planck Institute for Chemical Ecology, Jena, Germany*

TP 422 **Improved Quantification of Carbonyl Sub-metabolome by LC-MS Using a Fragmentation-Controlled Multiplexed Isotopic Tag**; Xiaobo Tian[1]; Gérard Hopfgartner[1]; *[1]University of Geneva, Geneva, Switzerland*

TP 423 **Identification of Anatoxin-a and Relevant Metabolites in Biological Matrices with High Resolution Mass Spectrometry**; Taylor J Glattke[1]; Mike A Mojica[2]; Logan C Krajewski[2]; Kirsten A Cottrill[1]; Brady R Cunningham[2]; Sarah R Lagon[1]; Brenda Ruto[3]; Donna Hill[4]; Elizabeth I Hamelin[2]; *[1]Battelle Memorial Institute, Atlanta, GA; [2]U.S. Centers for Disease Control and Prevention, Atlanta, GA; [3]Oak Ridge Institute for Science and Education, Oak Ridge, TN; [4]U.S. Environmental Protection Agency, Research Triangle Park, NC*

TP 424 **Small Molecule Retention Time Prediction for Nanoflow Liquid Chromatography using a Novel Machine Learning Approach**; Matthew Turner[1]; Luke Durell[1]; Sean Colby[1]; Sydney Schwartz[1]; Eva Brayfindley[1]; Anna Hale[1]; Jessica Bade[1]; Fanny Chu[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TP 425 **Discovering and annotating new molecules in untargeted metabolomics through structural coupling**; Shipei Xing[1, 2]; Yasin El Abiead[1, 2]; Abubaker Patan[1]; Paulo Wender Portal Gomes[1, 2]; Simone Zuffa[1, 2]; Helena Mannochio-Russo[1, 2]; Ipsita Mohanty[1, 2]; Pieter C. Dorrestein[1, 2]; *[1]UC San Diego, La Jolla, CA; [2]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

TP 426 **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[1]; Elizabeth T Anderson[1]; John S Ramsey[2]; Kevin B Hernandez[3]; Yong Yang[2]; Zachary Stansell[3]; Tyler Gordon[3]; Theodore W Thannhauser[2]; Sheng Zhang[1]; *[1]Proteomics and Metabolomics Facility, Cornell University, Ithaca, NY; [2]R.W. Holley Center for Agriculture and Health, USDA-ARS, Ithaca, NY; [3]Plant Genetic Resources Unit, USDA-ARS, Geneva, NY*

TP 427 **Comprehensive scoring system for high-confidence lipid identification in untargeted lipidomics**; Rui Qin[1]; William Xu[1]; Adriana Zardini Buzatto[2]; Elvis Lo[1]; Shuang Zhao[1]; Liang Li[1, 3]; *[1]The Metabolomics Innovation Centre, Edmonton, AB; [2]University of Calgary, Calgary, AB; [3]University of Alberta, Edmonton, AB*

TP 428 **Forward and Reverse Cosine Similarity Scoring During Real-Time Library Search for Triggering Additional Experiments on Indole Compounds in Plant Extract**; Brandon Bills[1]; Michael W Christopher[2]; Sunandini Yedla[1]; Bashar Amer[1]; Susan S Bird[3]; Rahul Deshpande[1]; William Barshop[1]; Boone M. Prentice[2]; Timothy J. Garrett[2]; Vlad Zabrouskov[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of Florida, Department of Chemistry, Gainesville, FL; [3]Thermo Fisher Scientific, Remote, MS*

TP 429 **Enabling Combined Qualitative/Quantitative CE-MS Metabolomics with Migration Time Indexing, Simplified Extraction, and a Novel Discovery Feedback Loop**; J. Will Thompson[1]; Erin A. Redman[1]; Scott Mellors[1]; Sam Stewart[2]; Joshua P. Guerrette[1]; Chrisopher D. Brown[2]; *[1]908 Devices Inc, Morrisville, NC; [2]908 Devices Inc., Boston, MA*

TP 430 **The Shin-MassBank project: Enrichment of MassBank records using human metabolome datasets**; Fumio Matsuda[1]; Aykiyoshi Hirayama[2]; Ryosuke Hayasaka[2]; Masatomo Takahashi[3]; Akiyasu C. Yoshizawa[4]; Kozo Nishida[5]; Taihei Torigoe[3]; Takato Kiuchi[4]; Yuki Matsuzawa[5]; Hiroshi Tsugawa[5]; Shujiro Okuda[4]; Yoshihiro Izumi[3]; *[1]Osaka Univeristy, Suita, Japan; [2]Keio University, Tsuruoka, Japan; [3]Kyushu University, Fukuoka, Japan; [4]Niigata University, Niigata, Japan; [5]Tokyo University of Agriculture and Technology, Koganei-shi, Japan*

TP 431 **Characterization of Glucosinolates in Arabis sagittata Extracts using a Multi-Reflecting Q-Tof Mass Spectrometer**; Emma Marsden-Edwards[1]; Sabine Metzger[2]; Martin Palmer[1]; Isabel Riba[1]; Vera Wewer[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]University of Cologne, Cologne, Germany*

TP 432 **Metabolic Profile of 25E-NBOH in Human Liver Microsomes, Rat Urine and Cunninghamella elegans**; Magdalena Vagnerova[1, 2]; Monika Mrnava[1]; Petr Palivec[1]; Bronislav Jurasek[1]; David Sykora[2]; Martin Kuchar[1]; *[1]Forensic Laboratory of Biologically Active Substances, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic; [2]Department of Analytical Chemistry, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic*

TP 433 **Advanced Mass Spectrometry Workflows for Novel Fragmentation Approaches for Small Molecule Agrochemical Applications**; Chris J Brown[1]; J.C. Yves LeBlanc[2]; Mircea Guna[2]; Yelena Adelfinskaya[3]; Jesse Balcer[3]; Jeffrey R Gilbert[3]; *[1]Corteva Agrisciences, Indianapolis, IN; [2]SCIEX, Concord, ON; [3]Corteva Agriscience, Indianapolis, IN*

METABOLOMICS: SAMPLE PREPARATION
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TP 434 **Exploring extraction methods for an combined metabolomic and proteomic analysis of potato tubers using high resolution mass spectrometry**; Pierre Otuszewski; *University of Lille, Villeneuve D'Ascq, France*

TP 435 **Salt Concentration in Sample Preparation has Variable Effects on Polar Feature Detection in Non-Targeted LC-MS Experiments**; David A Gaul[1]; Ying Liu[1]; Samuel G Moore[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

TP 436 **SWipe: Low-Cost Fecal Metabolome Sampling**; Alexey Melnik[1, 2]; Alexander Aksenov[1, 2]; *[1]University of Connecticutt, Storrs, CT; [2]Arome Science Inc., Farmington, CT*

TP 437 **Expanding metabolic coverage for sustained large-scale reversed-phase profiling of blood products using a novel dispersive solid phase extraction protocol**; Mark David[1]; Elena Chekmeneva[1]; Maria Gomez Romero[1]; Stephane Camuzeaux[1]; Benjamin Cooper[1]; Ada Armstrong[1]; Ravi Mehta[1]; Shiranee Sriskanda[1]; Miguel Reis Ferreira[2]; Olivier Cloarec[3]; Caroline Sands[1]; Goncalo Correia[1]; Zoltan Takats[1]; Matthew R Lewis[1]; *[1]Imperial College London, London, United Kingdom; [2]King's College London, London, United Kingdom; [3]Sartorius Stedim Biotech GmbH, Goettingen, Germany*

TP 438 **Automated sample preparation using the Waters Andrew+ pipetting robot with biocrates' MxP®Quant 500 kit for high-throughput metabolomic profiling.**; Zachary J Mayer[1]; Stephen Dearth[2]; Timothy Griffin[1]; Giorgio Horak[3]; Vincent Bel[3]; Markus Langsdorf[2]; Candace Guerrero[1]; *[1]Center for Metabolomics and Proteomics, University of Minnesota, Minneapolis, MN; [2]biocrates life sciences ag – Eduard-Bodem-Gasse 8, Innsbruck, Austria; [3]Waters Corporation, Eschborn, Germany*

TP 439 **Mass Spectrometry Detection of Root Exudate Metabolites by Filter Based Sampling**; Nilay Saha[1]; Alessandra Ceretto[1]; Cynthia Weinig[1]; Franco Basile[1]; *[1]University of Wyoming, Laramie, WY*

TP 440 **Easy-‘Omics: Taking the sweat out of metabolomics through automation**; Joshua P. Guerrette[1]; Erin Redman[1]; Scott Mellors[1]; Sam Stewart[1]; J. Will Thompson[1]; *[1]908 Devices Inc, Morrisville, NC*

TP 441 **Sample Preparation Optimization for Metabolomics Analysis of Cell Culture Media to Reduce Maillard Reaction Products**; Vyncent Nguyen[1]; Didar Asik[1]; Andy Campbell[1]; Jaime S Goldfuss[1]; Chengjian Tu[1]; *[1]Thermo Fisher Scientific, Buffalo, NY*

TP 442 **---Extraction conditions impact recovery of specific metabolites in murine samples**; Amy Johnson[1]; Molly T. Soper-Hopper[1]; Rachel J. House[1]; Michael P. Vincent[1]; Abigail E. Ellis[2]; Christine N. Isaguirre[2]; Ryan D. Sheldon[2];

[1]Van Andel Research Institute, Grand Rapids; [2]Van Andel Research Institute, Grand Rapids, MI

TP 443 **High-Throughput and Low-Input Metabolomics/Lipidomics Sample Preparation – A New BeatBox® Application**; Cameron Ellis[1]; Bryan Ngo[2]; Daniel Itzhak[2]; Junhua Wang[2]; Katharina Limm[3]; *[1]PreOmics, Billerica, MA; [2]Altos Labs, Redwood City, California; [3]PreOmics GmbH, München, Germany*

TP 444 **Evaluation of Metabolomics of Dried Blood from Various Remote Sampling Technologies: Parameters of Acquisition, Extraction and Analysis**; Jiajun Lei[1]; Jonathan E. Katz[1, 2]; *[1]Ellison Institute of Technology, Los Angeles, CA; [2]University of Southern California, Los Angeles, CA*

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TP 445 **Metabolomics-aided biomarker discovery and elucidationof molecular pathways**; Anthony Tsarbopoulos[1]; Nikolaos Stavros Koulakiotis[2]; Evangelia Karkoula[2]; Ioanna Dagla[2]; Evagelos Gikas[1]; Nikolaos Kokras[1]; Christina Dalla[1]; *[1]National and Kapodistrian University of Athens Medical School, Athens, Greece; [2]The Goulandris Natural History Museum, Kifissia, Greece, Kifissia, Greece*

TP 446 **Differential Metabolomics for Mouse Liver Induced by Microplastics Utilizing SWATH-based Mass Spectrometry**; Kuan-Lu Wu[1]; Sung-Fang Chen[1]; *[1]National Taiwan Normal University, Taipei, Taiwan*

TP 447 **LC-MS/MS reveals kelp forest DOM composition and key insights into how algae exudates influence species interactions**; Shane Farrell[1]; Daniel Petras[2]; Dara Yiu[1]; Abzer K Pakkir Shah[3]; Aaron Hartmann[4]; John Burns[1]; Damian Brady[5]; Doug Rasher[1]; *[1]Bigelow Laboratory for Ocean Sciences, East Boothbay, ME; [2]University of California Riverside, Department of Biochemistry, Riverside, CA; [3]University of Tuebingen, Center for Plant Molecular Biology, Tübingen, Germany; [4]Harvard University, Cambridge, MA; [5]University of Maine, Darling Marine Center, Walpole, ME*

TP 448 **Elucidating the protective mechanisms of oral hyaluronic acid against UV-induced skin damage: a metabolomic and lipidomic approach**; Matej Simek[1]; Vratislav Berka[1]; Lukáš Opálka[2]; Martina Bajerová[3]; Kateřina Lehká[1]; Iva Dolečková[1]; Lukáš Kubala[3]; *[1]Contipro, Dolni Dobrouc, Czech Republic; [2]Faculty of Pharmacy, Hradec Králové, Czech Republic; [3]Institute of Biophysics, Brno, Czech Republic*

TP 449 **Untargeted LC-HRMS-based metabolomic profiling reveals distinct metabolomic profiles in patients with metabolic dysfunction-associated steatotic liver disease**; Qing Zhao[1]; Guoshou Teo[1]; Pradeep Narayanaswamy[2]; Will De Nardo[3]; Umur Keles[4]; Philipp Kaldis[4]; Matthew Watt[3]; Hyungwon Choi[1]; *[1]National University of Singapore, Singapore, Singapore; [2]SCIEX, Singapore, Singapore; [3]The University of Melbourne, Melbourne, Australia; [4]Lund University, Lund, Sweden*

TP 450 **Feature Agnostic Metabolomics for Dose Range Finding Experiments in Sub-cytotoxic Doses of Common Pesticides in Primary Human Cells**; Madison Grace Thornhill[1, 2]; Emilio S. Rivera[1, 2]; Erick S. LeBrun[1, 2]; Emilia A. Solomon[2]; Claire K. Sanders[3]; Tara Harvey[1, 2]; Joshua D. Breidenbach[1, 2]; Brett R. Blackwell[1, 2]; Marc Alvarez[2]; Kes A. Luchini[1, 2]; Abigale S Mikolitis[1, 2]; Zachary J. Sasiene[1, 2]; Ethan M. McBride[1, 2]; Austin R. Anderson[1, 2]; Lauren K. Heine[1, 2]; Chi-Yen Tseng[1, 2]; Jessica A. Salguero[1, 2]; Francisca E. Rodriguez[1, 2]; Salvator J. Palmisano[1, 2]; Jeremy Norris[4]; Phillip M. Mach[1, 2]; Trevor G. Glaros[1, 2]; *[1]Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [2]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [3]Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN*

TP 451 **Metabolomic Fingerprint of Leishmaniasis: Profiles of Cutaneous and Mucosal Leishmania species with and without endosymbiotic Leishmania RNA Virus (LRV).**; Joseane L P G Pavao[1, 2]; Andrea Lafleur[3]; Mahbobeh Lesani[2]; Martin Olivier[3]; Laura-Isobel McCall[1, 2]; *[1]San Diego State University, San Diego, CA; [2]University of Oklahoma, Norman, OK; [3]The Research Institute of the McGill University Health Centre, Infectious Diseases and Immunity in Global Health Program, Montreal, Quebec*

TP 452 **Characterizing UVPD and HCD Fragmentation Patterns of Diverse Indolic Small Molecules to Aid in Surveying the "Indolome"**; Michael W Christopher[1]; Sunandini Yedla[2]; Bashar Amer[2]; Susan Bird[2]; Rahul Deshpande[2]; William Barshop[2]; Boone M. Prentice[1]; Brandon Bills[2]; Timothy J. Garrett[1]; *[1]University of Florida Department of Chemistry, Gainesville, FL; [2]Thermo Fisher Scientific, San Jose, CA*

TP 453 **A Novel Approach for Comprehensive Carboxylic Acid Profiling Utilizing Halogenated Derivatization and Liquid Chromatography-Trapped Ion Mobility Spectrometry-Mass Spectrometry**; Kaylie I. Kirkwood-Donelson[1]; Prashant Rai[1]; Michael B. Fessler[1]; Alan K. Jarmusch[1]; *[1]National Institute of Environmental Health Sciences, Durham, NC*

TP 454 **Rapid Assessment of Metabolism by Electrochemistry/MS -Drugs, Xenobiotics, Plants**; Martin Eysberg[1]; Hendrik-Jan Brouwer[2]; Jean-Pierre Chervet[2]; *[1]Antec Scientific, LLC, Boston, MA; [2]Antec Scientific, Alphen aan den Rijn, Netherlands*

TP 455 **Characterization of steroid conjugates by LC-MS/MS using collision-induced dissociation, electron activated dissociation and UV-photodissociation**; Lysi Ekmekciu[1]; Gérard Hopfgartner[1]; *[1]University of Geneva, Genéve, Switzerland*

TP 456 **FERMENTATION SUBSTRATE OPTIMIZATION UTILIZING COMPARATIVE ANALYSES CAPABILITY OF DIFFERENT METABOLOMIC PLATFORMS**; Garima Agarwal[1]; Jeremy McFadden[1]; Chris Brown[1]; Michael Fethe[1]; *[1]Corteva Agrisciences, Indianapolis, IN*

TP 457 **A Comprehensive Analysis of Monozygous and Dizygous Twin Pairs discordant for Type 1 Diabetes (T1D) through LC-MS/MS Metabolomics**; Elizabeth R Flammer[1]; Hali C. Broncucia[2]; Andrea K. Steck[2]; Stephen E. Gitelman[3]; Heba M. Ismail[4]; Timothy J. Garrett[1]; *[1]University of Florida, Department of Chemistry, Gainesville, FL; [2]Barbara Davis Center for Diabetes, University of Colorado Anschutz Medical Campus, Aurora, CO; [3]Department of Pediatrics, Diabetes Center, University of California at San Francisco, San Francisco, CA; [4]Department of Pediatrics, Indiana University School of Medicine, Indianapolis, IN*

TP 458 **Molecular changes of stained teeth by hydrogen peroxide and peroxymonosulfate treatments**; Paulo Wender Portal Gomes[1]; Simone Zuffa[1]; Anelize Bauermeister[1]; Andrés Mauricio Caraballo-Rodríguez[1]; Haoqi Nina Zhao[1]; Helena Mannochio-Russo[1]; Cajetan Dogo-isonagie[2]; Om Patel[2]; Paloma Pimenta[2]; Jennifer Gronlund[2]; Stacey Lavender[2]; Shira Pilch[2]; Venda Maloney[2]; Michael North[2]; Pieter C. Dorrestein[1]; *[1]University of California San Diego, La Jolla, CA; [2]Colgate-Palmolive, Piscataway, NJ*

TP 459 **Selecting Optimal Internal Standards for Non-targeted LC-MS Metabolomics in a Large Core Facility**; Emilia J McCann[1]; Uri Keshet[1]; Oliver Fiehn[1]; *[1]University of California Davis, Davis, CA*

TP 460 **A comprehensive Untargeted Fecal Metabolomics Workflow on the Orbitrap Astral MS to Achieve Deep Metabolome Coverage and Confident Compound Annotation**; Bashar Amer[1]; Yasin El Abiead[2]; Pieter C. Dorrestein[2]; Daniel Hermanson[1]; Susan Bird[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of California - San Diego, San Diego, California*

TP 461 **Demystifying microbore UHPLC-HRMS for sensitive and robust untargeted metabolomics**; Eduardo Sommella[1]; Danila La Gioia[1, 2]; Pietro Campiglia[1]; *[1]University of Salerno, Fisciano (SA), Italy; [2]PhD Program in Drug Discovery and Development, University of Salerno, Fisciano, SA, Italy, Fisciano (SA), Italy*

TP 462 **Metabolomic Profiling of Osteocyte Extracellular Vesicles and Matrix Bound Vesicles using a Prototype Benchtop Multi Reflecting Time-of-Flight (MRT) Mass Spectrometer**; Lisa Reid[1]; Alicia Keenan[2]; Stephen Griffin[3]; Lee A Gethings[1]; Liam M Heaney[2]; Aveen Jalal[2]; Genevieve Anghileri[2]; Owen G Davies[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]School of Sport, Exercise and Health Sciences, Loughborough University, Loughborough, United Kingdom; [3]Waters Corporation, Milford, Massachusetts*

TP 463 **Development of microfluid based UPLC-MS untargeted metabolomic methods for newborn screening**; Etienne Ljoni Poisson[1]; Freyr Jóhansson[2]; Leifur Franzson[3]; Margrét Þorsteinsdóttir[4]; Jón Jóhannes Jónsson[5]; Ottar Rolfsson[6]; *[1]University of Iceland, Reykjavik, Iceland; [2]Department of Genetics and Molecular Biology, Icelandic National Hospital, Reykjavik, Iceland; [3]Project Leader, Department of Clinical Biochemistry, Icelandic National Hospital, Reykjavik, Iceland; [4]Professor, Faculty of Pharmaceutical Sciences, University of Iceland, Director of R&D at ArcticMass, Reykjavik, Iceland; [5]Director of Genetics and Molecular Medicine, Icelandic National Hospital, Reykjavik, Iceland; [6]Professor at The Centre for Systems Biology, Medical School, University of Iceland, Reykjavik, Iceland*

TP 464 **Mass query language and collisional cross section prediction to support chemical derivatization research using mass spectrometry**; Jesba Bas Concepcion[1]; Jeffrey R Gilbert[2]; Chris Brown[2]; Sofie Weinkouff[3]; Dave Robbins[2]; Heiko Neuweger[3]; *[1]Corteva, Whitestown, IN; [2]Corteva Agriscience, Indianapolis, IN; [3]Bruker Daltonics GmbH & Co. KG, Billerica, MA*

TP 465 **Untargeted metabolomics reveals secondary metabolites associated with fungal-fungal competition under select nutrient conditions**; Sameer Mudbhari[1, 2]; Jose Eduardo Marques Galvez[3]; Claire Veneault-Fourrey[3]; Robert L Hettich[1, 2]; Paul E Abraham[1, 2]; *[1]The University of Tennessee Knoxville, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]INRAE-Université de Lorraine, Nancy, France*

TP 466 **Untargeted metabolomic profiling reveals process optimization strategies in a mock bioreactor**; Adam D Richardson[1]; Ethan Stancliffe[1]; Monil Gandhi[1]; Ashima Mehta[1]; Kevin Y Cho[2]; Gary J. Patti[1, 2]; *[1]Panome Bio, St Louis, MO; [2]Washington University in St. Louis, St. Louis, MO*

TP 467 **Optimization of sample preparation and LC-MS analysis for high-throughput untargeted lipidomics and metabolomics**; Djawed Bennouna[1]; Christopher A LeClair[1]; Ewy Mathé[1]; *[1]NIH/NCATS, Rockville, Maryland*

TP 468 **Expanding Normalization Coverage using Surrogate Metabolites in the Human Cell Metabolome**; Olivia Taverniti[1]; Brandon Y Lieng[1]; Jeremy K Chan[1]; William D Gwynne[1]; Andrew T Quaile[1]; J. Rafael Montenegro-Burke[1]; *[1]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON*

TP 469 **Metabolomics and lipidomics approaches for the identification of HCC biomarkers in patients with liver cirrhosis**; Md Mamunur Rashid[1]; Rency S Varghese[1]; Habtom Ressom[1]; *[1]Georgetown University, Washington, DC*

TP 470 **Untargeted Metabolomics for Differential Analysis of Bacterial-Induced Sepsis**; Michael P Napolitano[1]; Hong Wang[1]; Bruce A Kimball[1]; *[1]Monell Chemical Senses Center, Philadelphia, PA*

TP 471 **Simultaneous Quantitation and Discovery (SQUAD) Liquid Chromatography Mass Spectrometry of Progesterone Steroids Relevant to Ovarian Cancer**; Elisabeth Schwiebert[1]; Samuel G. Moore[1, 2]; Jaeyeon Kim[3]; David A. Gaul[1, 2]; Facundo M. Fernández[1, 2]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Altanta, GA; [2]Petit Institute of Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA; [3]Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indiana University, Melvin and Bren Simon Comprehensive Cancer Center, Indianapolis, IN*

TP 472 **Juicy Insights: A Nontargeted, Standardized Metabolomics Approach for Comparing Apples to Apples**; Melanie Odenkirk[1, 2]; Margaret Read[1]; Cole Michel[3]; Katrina Doenges[3]; Jacqueline Michelle Chaparro[1]; Susan B Mitchell[1]; Nathan Montgomery[1]; Corey D Broeckling[1]; Sarah Brinkley[4]; Katrina L Leaptrot[5]; Stacy D Sherrod[5]; Jody C May[5]; Juliana Chaura[6]; Gabriel E Velez Mejia[6]; Arpana Vaniya[7]; John A McLean[5]; Richard Reisdorph[3]; Nichole Reisdorph[3]; Andres Jaramillo-Botero[6, 8]; Oliver Fiehn[7]; Chi-Ming Chien[2]; Tracy Shafizadeh[2]; Jessica E Prenni[1]; Steve Watkins[2]; *[1]Colorado State University, Fort Collins, CO; [2]Verso Biosciences, Davis, CA; [3]University of Colorado, Anschutz Medical Campus, Department of Pharmaceutical Sciences, Aurora, CO; [4]The Alliance of Bioversity International & The International Center for Tropical Agriculture (CIAT), Cali, Colombia; [5]Vanderbilt University, Nashville, TN; [6]Pontificia Universidad Javeriana, Cali, Colombia; [7]University of California, Davis, Davis, California; [8]California Institute of Technology, Pasadena, CA*

TP 473 **High throughput plasma profiling of human liver disease samples using rapid chromatography and a multi-reflecting time-of-flight mass spectrometer**; Adam M King[1]; Ana S Lorenzo[2]; Yuriy Pyatkivskyy[3]; Emma Marsden-Edwards[1]; Elizabeth J Want[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Imperial College London, London, United Kingdom; [3]Waters Corporation, Milford, Massachusetts*

TP 474 **Exploring Metabolites within Organoids and Organoids-on-Chips during Colorectal Cancer (CRC) Therapeutic Treatments**; Ethan Canfield[1]; Carly Strelez[1]; Rachel Perez[1]; Aaron Schatz[1]; Heinz-Josef Lenz[2]; Jonathan Katz[1]; Shannon Mumenthaler[1]; *[1]Ellison Institute of Technology, Los Angeles, CA; [2]University of Southern California, Los Angeles, CA*

TP 475 **Advancing Metabolomics Analysis using GC-MS with Cold EI for Increased Identification, Throughput, and Sensitivity**; Luis M Valdiviez[1]; Uri Keshet[1]; Aviv Amirav[2]; Benjamin Neumark[2]; Oliver Fiehn[1]; *[1]West Coast Metabolomics Center, University of California, Davis, Davis, CA; [2]Tel Aviv University, Tel Aviv, Israel*

TP 476 **A Multi-Omic Identification Protocol for High-Throughput Bacterial Analysis**; Jana M Carpenter[1]; Hannah Hynds[1]; Kingsley Bimpeh[1]; Kelly M. Hines[1]; *[1]University of Georgia, Athens, GA*

TP 477 **Utilizing liquid chromatography and mass spectrometry techniques for metabolic profiling of citrus parental varieties to inform breeding strategies** ; Anil Bhatia[1]; Pallavi Agarwal[2]; Manhoi Hur[1]; Amancio J De Souza[1]; Chandrika Ramadugu[2]; *[1]UCR Metabolomics Core, University of California, Riverside, California; [2]Department of Botany and Plant Sciences, University of California, Riverside, CA*

TP 478 **Untargeted Exploration of Putative Emotional Chemo-Signals by thermal desorption preconcentration GC-EI&CI-TOFMS**; Marleen Vetter[1]; Eliska Ceznerova[1]; Sonja Klee[1]; Steffen Bräkling[1]; Megan Claflin[2]; Biagio D`Aniello[3]; Alfredo Di Lucrezia[3]; Anna Scandurra[3]; Claudia Pinelli[4]; Francesco Loreto[5]; Maurilia M. Monti[6]; Michelina Ruocco[6]; Gün R. Semin[7]; Luca Cappellin[8]; *[1]TOFWERK, Thun, Switzerland; [2]Aerodyne Research Inc., Billerica, MA; [3]Univeristy of Naples Federico II, Napels, Italy; [4]University of Campania Luigi Vanvitelli, Caserta, Italy; [5]University of Naples Federico II, Napels, Italy; [6]Italian National Research Council (CNR), Naples, Italy; [7]William James center of research ISPA, Lisbon, Portugal; [8]University of Padua, Padua, Italy*

MICROORGANISMS AND THE MICROBIOME II

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TP 479 **MftP is a Multi-Drug Efflux Pump with a Vital Role in Regulating Cellular Homeostasis in Burkholderia thailandensis**; Ahmed Al-Tohamy[1]; Fabrizio Donnarumma[1]; Anne Grove[1]; *[1]Louisiana State University, Baton Rouge, LA*

TP 480 **Spent media analysis and metabolic modeling-guided bioprocess optimization for recombinant protein production from E. colion complex media**; Hardik Dodia[1]; Vivek Mishra[2]; Charandatta Muddana[2]; Prajval Nakrani[2]; Pramod P. Wangikar[1, 2]; *[1]Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai, India; [2]Clarity Bio Systems India Pvt. Ltd., Pune, India*

TP 481 **MetaLab: An Advanced Software Solution for Comprehensive DDA and DIA Metaproteomics Analysis on Multiple MS Platforms**; Kai Cheng[1]; Zhibin Ning[1]; Daniel Figeys[1]; *[1]University of Ottawa, Ottawa*

TP 482 **Plasma metabolomics uncovers characteristic metabolic aberrancies in early-onset Crohn's Disease**; Zhiwei Zhou[1]; Yuanyuan Liu[1]; Ruben Colman[1]; Michael Rosen[1]; Michael Fischbach[1]; Dylan Dodd[1]; *[1]Stanford University, Stanford, CA*

TP 483 **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[1]; Yanlin Shi[1]; Jihyun Park[1]; *[1]Produce Safety & Microbiology, Western Regional Research Center, Agricultural Research Service, USDA, Albany, CA*

TP 484 **The impact of MALDI-TOF-MS sampling rates on microbial identification results**; Ko Keng Chang[1]; Yi-Sheng Wang[1]; *[1]Academia Sinica, Taipei, Taiwan*

TP 485 **A Simplified and Efficient Method for Expanding Gut Metaproteomic Coverage**; Pei-Chen Hsu[1]; Pei-Shan Wu[2]; Chuan-Chih Hsu[3]; Miao-Hsia Lin[4]; *[1]Department of Microbiology, College of Medicine, National Taiwan University, Taipei City, Taiwan; [2]Department of Ophthalmology, National Taiwan University Hospital, College of Medicine, National Taiwan University, Taipei city, Taiwan; [3]Institute of Plant and Microbial Biology, Academia Sinica, Taipei city, Taiwan; [4]Department of Microbiology, College of Medicine, National Taiwan Univeristy, Taipei city, Taiwan*

TP 486 **Applying Untargeted Metabolomics to a Synthetic Cystic Fibrosis Microbial Community**; Emily C Giedraitis[1]; Rachel L Neve[2]; Vanessa V Phelan[1]; *[1]Department of Pharmaceutical Sciences, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of Colorado-Anschutz Medical Campus, Aurora, CO; [2]Department of Immunology and Microbiology, School of Medicine, University of Colorado-Anschutz Medical Campus, Aurora, CO*

TP 487 **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[1]; Michael Russelle S. Alvarez[1]; Luiz Eduardo Lacerda[2]; Ricardo Wagner Portela[2]; Carlito B. Lebrilla[1]; *[1]University of California Davis, Davis, CA; [2]Universidade Federal da Bahia, Salvador, Brazil*

TP 488 **Protein O-glycosylation in the Bacteroidota phylum**; Dennis Svedberg[1]; Elisabeth Baland[1]; Lucía Perez[1]; Bolor Buyanbadrakh[1]; Shaochun Zhu[1]; Andre Mateus[1]; *[1]Umeå University, Umeå, Sweden*

TP 489 **De Novo Library Construction for Metaproteomic Analyses of Human Datasets**; Andrew T Rajczewski[1]; Reid Wagner[2]; Subina P Mehta[1]; Tim Griffin[1]; Pratik Dilip Jagtap[1]; *[1]University of Minnesota, Twin Cities, Minneapolis, MN; [2]Minnesota Supercomputing Institute, Minneapolis, MN*

TP 490 **Structural characterization of commensal bacteria-derived lipid As and elucidation of their impact on host immune responses**; Byoungsook Goh[1]; Ji-Sun Yoo[1]; Sungwhan F. Oh[1, 2]; *[1]Brigham and Women's Hospital, Boston, MA; [2]Harvard Medical School, Boston, MA*

TP 491 **Changes in Infant Health-Related Metabolites during Pregnancy After a Nutritional Intervention**; Emma R Guiberson[1]; Elisa Caffrey[1]; Justin L Sonnenburg[1, 2, 3]; *[1]Department of Microbiology and Immunology, Stanford University, Palo Alto, California; [2]Chan-Zuckerburg Biohub, San Francisco, California; [3]Center for Human Microbiome Studies, Stanford University, Palo Alto, CA*

TP 492 **Bacterioscore in 2D/3D MS imaging: pioneering in vivocancer microbiome study and its link with diagnosis and patient survival**; Léa LEDOUX[1]; Yanis Zirem[1]; Michel Salzet[1]; Isabelle Fournier[1]; *[1]PRISM - Inserm U1192, Villeneuve d'Ascq Cedex France, France*

TP 493 **Multi-omic network analysis identifies synergistic mechanisms for dietary lipids and microbiome pathobionts to drive macrophage innate immunity and metabolic disease**; Jacob W Pederson[1, 2]; Jyothi Padiadpu[2]; Andrey Morgun[2]; Natalia Shulzhenko[2]; Aleksandra Nita-Lazar[1]; *[1]NIAID, Bethesda, MD; [2]Oregon State University, Corvallis, OR*

TP 494 **Development of novel mouse models with improved translatability to the human microbiome**; Szymon Filip[1]; Greg Fedewa[1]; Cuong Nguyen[1]; Leslie Sedgeman[1]; Jasmine Chong[1]; Antonio Carmona[1]; Miriam Velez[1]; Nathan Wan[1]; Yan Yang[1]; Sarkis Mazmanian[2]; Bryan Yoo[1]; *[1]Nuanced Health, Los Angeles, CA; [2]California Institute of Technology, Pasadena, CA*

TP 495 **A multimodal platform for lipid A structural analysis from a single colony**; Hyojik Yang[1]; Ian O'Keefe[1]; Richard D. Smith[1]; Kylie P. Sumner[1]; Matthew E. Sherman[1]; DAVID R GOODLETT[2]; Charles R. Sweet[3]; ROBERT K ERNST[1]; *[1]University of Maryland, Baltimore, MD; [2]University of Victoria, Victoria, BC; [3]United States Naval Academy, Annapolis, MD*

TP 496 **Beyond the Biotyper: leveraging LC-MS proteomics to systematically map the proteomes of 38,000 bloodstream infection isolates**; Annegret Ulke-Lemee[1]; Rory Gilliland[1]; Mario Valdés-Tresanco[1]; Morgan Hepburn[1]; Ryan Groves[1]; Anika Westlund[1]; Andriy Plakhotnyk[1]; Gopal Ramamourthy[1]; Daniel Gregson[2]; Thi Mui Pham[3]; Tatum Mortimer[4]; Joshua Smith[5]; Bruce Walker[5]; Yonatan Grad[3]; Ashlee Earl[5]; Hallgrimur Benediktsson[1]; Ethan MacDonald[1]; Ian Lewis[1]; *[1]University of Calgary, Calgary, AB; [2]Alberta Provincial Laboratories, Calgary, AB; [3]Harvard T.H. Chan School of Public Health, Boston, MA; [4]University of Georgia, Athens, GA; [5]Broad Institute, Cambridge, MA*

TP 497 **Stabilizing the Mycobacterial Small Proteome Through Proteasome Inhibition**; Hannah A. Marietta[1]; Simon D Weaver[1]; Taylor J. Lundgren[1]; Patricia L. Clark[1]; Matthew M. Champion[1]; *[1]University of Notre Dame, Notre Dame, IN*

TP 498 **LC-MS as a platform for precision medicine: predicting survival from bloodstream infections using a training set of 38,000 microbial proteomes**; Rory Gilliland[1]; Ashlee Earl[2]; Anika Westlund[1]; Bruce Walker[2]; Andriy Plakhotnyk[1]; Annegret Ulke-Lemee[1]; Colin Mackenzie[1]; Morgan Hepburn[1]; Thi Mui Pham[3]; Gopal Ramamourthy[1]; Yonatan Grad[3]; Hallgrimur Benediktsson[1]; Ethan MacDonald[1]; Ian Lewis[1]; *[1]University of Calgary, Calgary, AB; [2]Broad Institute, Cambridge, MA; [3]Harvard T.H. Chan School of Public Health, Boston, MA*

TP 499 **Application of a microbiome-specific metabolite library in untargeted plasma metabolomics**; Jaclyn Weinberg[1]; William Crandall[1]; Anthony Gacasan[1]; Sami Teeny[1]; James Zhan[1]; Rheinallt Jones[1]; Michael Woodworth[1]; Dean Jones[1]; *[1]Emory University, Atlanta, GA*

TP 500 **The virus microenvironment in 2D and 3D: Intercellular communication guides tumor-specific vulnerabilities to viral infection**; Krystal K. Lum[1]; James C. Kostas[1]; Colter Brainard[1]; Oscar Pundel[2]; Qingwen Jiang[3]; Karuna Ganesh[3]; Benjamin G. Neel[2]; Ileana M. Cristea[1]; *[1]Princeton University, Princeton, NJ; [2]NYU Langone, New York, NY; [3]Memorial Sloan Kettering Cancer Center, New York, NY*

TP 501 **From Dirt to Data: Comparing Liquid Chromatography-Mass Spectrometry Methods for Low-Biomass Soil**

Metaproteomics; Dorathea Lee[1]; Gustavo Diaz[1]; Valerie A Seitz[2]; Mikayla A Borton[3]; Meagan E Schipanski[3]; Jessica E Prenni[2]; Kelly C Wrighton[3]; Corey D Broeckling[1]; *[1]Analytical Resources Core: Bioanalysis and Omics Center, Colorado State University, Fort Collins, CO; [2]Department of Horticulture and Landscape Architecture, Fort Collins, CO; [3]Department of Soil and Crop Sciences, Colorado State University, Fort Collins, CO*

TP 502 **Aspergillus fumigatus secretes gliotoxin in response to polymycovirus infection**; Rutuja H Patil[1]; Amer Ali Abd El-Hafeez[2]; Gabriele Sass[3]; David A. Stevens[2]; Andrea Palyzová[4]; Joe Hsu[2]; Ioly Kotta-Loizou[5]; Vladimír Havlíček[1]; *[1]Institute of Microbiology of the Czech Academy of Sciences, 142 20, Prague, Czech Republic; [2]Stanford University, Stanford, CA; [3]California Institute for Medical Research, San Jose, CA; [4]Institute of Microbiology of the Czech Academy of Sciences, Prague, Czech Republic; [5]Imperial College London, London, United Kingdom*

TP 503 **A Targeted Multi-Omics Platform for Characterizing Prebiotic-Probiotic Interactions**; Christopher Suarez[1]; Cheng-Yu Charlie Weng[1]; Karen Kalanetra[2]; Sarah Blecksmith[3]; Danielle Lemay[3]; David A. Mills[2]; Carlito B. Lebrilla[1]; *[1]Department of Chemistry, University of California, Davis, Davis, California; [2]Department of Food Science and Technology, University of California Davis, Davis, CA; [3]Department of Nutritional Biology, University of California, Davis, Davis, CA*

NANOSCALE/MICROFLUIDIC AND CAPILLARY ELECTROPHORESIS SEPARATIONS AND MS

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TP 504 **Rapid Comparative Analysis of Glatiramer Acetate Products with CZE-MS**; Joshua Shipman[1]; A M Abdullah[1]; Cynthia Sommers[1]; Jason Rodriguez[1]; *[1]Office of Pharmaceutical Quality Research, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Saint Louis, MO*

TP 505 **Comparing the merits of capillary electrophoresis versus microfluidic capillary electrophoresis in the bottom-up characterization of larger nucleic acids**; Daniele Rollo[1]; Daniele Fabris[1]; *[1]University of Connecticut, Storrs, CT*

TP 506 **Coupling icIEF to high-resolution mass spectrometry for in-depth characterization of complex protein charge heterogeneity**; Teresa Kwok[1]; Tia Chan[1]; Matthew Courtney[1]; Tong Chen[1]; Tao Bo[1]; *[1]Advanced Electrophoresis Solutions, Cambridge, ON*

TP 507 **Capillary Electrophoresis Miniature Mass Spectrometry System for Rapid and Sensitive Clinical Analysis**; Min Dang[1]; Jiexun Bu[2]; Junhan Wu[1]; Xiao Chen[3]; Wenpeng Zhang[3]; Zheng Ouyang[3]; *[1]PURSPEC Technology (China) Ltd., Suzhou, China; [2]PURSPEC Technology (Beijing) Ltd., Beijing, China; [3]Tsinghua University, Beijing, China*

TP 508 **Characterization of Adeno-Associated Virus Capsids by a Novel Capillary Isoelectric Focusing-Based Fractionation Method and Charge Detection Mass Spectrometry**; Jiaqi Wu[1]; Benjamin Draper[2]; Chris Heger[1]; *[1]Bio-Techne, San Jose, CA; [2]Megadalton Solutions, Bloomington, Indiana*

TP 509 **Coupling a 3D-Printed Herringbone Device to cVSSI-MS for Reaction Kinetic Studies**; Amanda DeVor[1]; Jing Wang[1]; Olanrewaju Awoyemi[1]; Sydney Anderson[1]; Peng Li[1]; Stephen J Valentine[1]; *[1]West Virginia University- C. Eugene Bennett Department of Chemistry, Morgantown, WV*

TP 510 **Mass spectrometry-based top-down proteomics in nanomedicine: proteoform-specific measurement of nanoparticle protein corona**; Amirhossein Sadeghi[1]; Ali Akbar Ashkarran[1]; Morteza Mahmoudi[1]; Liangliang Sun[1]; *[1]Michigan State University, East Lansing, MI*

TP 511 **A Workflow for Antibody Charge Variant Fractionation Enabling CZE-MS**; Jiaqi Wu[1]; Scott J Mellors[2]; Will McElroy[1]; Chris Heger[1]; *[1]Bio-Techne, San Jose, CA; [2]908 Devices Inc., Boston, MA*

TP 512 **Fractionation of Bispecific Antibody Charge Variants by MauriceFlex™ and their Identification by Mass Spectrometry**; Srinivasa Rao[1]; Andreas Nageli[2]; Chris Heger[1]; *[1]Bio-Techne, San Jose, CA; [2]Genovis AB, Kävlinge, Sweden*

TP 513 **Optimization of Capillary Electrophoresis Mass spectrometry for Carbene Chemical Footprinting Analysis**; Daoyang Chen[1]; Laurence Fayadat-Dilman[1]; Jason Hogan[1]; *[1]Merck, South San Francisco, CA*

TP 514 **Development of highly sensitive sheathless CE-MS method and application to small volume cell analysis**; Akiyoshi Hirayama[1, 2]; Kenichi Takahashi[1]; Tomoyoshi Soga[1]; *[1]Keio University, Tsuruoka, Japan; [2]INCEMS Technologies, Co. Ltd., Tsuruoka, Japan*

TP 515 **Robust Capillary Isoelectric Focusing-Mass Spectrometry Separations of Proteins**; Caitlin M. Kerr[1]; Olivia L. Schneider[1]; Bonnie J. Huge[1]; Matthew M. Champion[1]; *[1]University of Notre Dame, Notre Dame, IN*

TP 516 **Single-Cell Metabolomic Characterization via CE-NanoESI-MS with Nanoflow Sheath Liquid Interface**; Shuangshuang Chen[1]; Mike Knierman[2]; Stanislav Rubakhin[1]; Noah A. Bender[1]; Yash Nelavelli[1]; Jonathan V Sweedler[1]; *[1]University of Illinois Urbana Champaign, Urbana, IL; [2]Agilent Technologies, Santa Clara, CA*

TP 517 **On-demand Mass Spectrometry for Modern Biopharmaceutical Workflows**; Austin Culberson[1]; Mason A Chilmonczyk[1]; *[1]Andson Biotech Inc., Atlanta, GA*

NEUROSCIENCE AND NEURODEGENERATIVE DISEASE RESEARCH

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TP 518 **Quantification of brain cholesterol and cholesterol metabolites regulation during demyelination and remyelination in a genetic mouse model**; Hudihim MWDK Dedunupitiya[1]; Eden Parreno Go[1]; Nishama De Silva Mohotti[1]; Jenna Marie Williams[1]; Hiroko Kobayashi[1]; Rashmi Basavaraj Binjawadagi[1]; Heather Desaire[1]; Meredith Hartley[1]; *[1]University of Kansas, Lawrence, KS*

TP 519 **Probabilistic graphical modeling approaches identify disease-specific features within complex lipidomic data from Parkinson's disease patient specimens**; Nathan G. Hatcher[1]; Dimitris V. Manatakis[1]; Nanyan R. Zhang[1]; Lihang Yao[1]; Cheryl E. G. Leyns[1]; Matthew J. Fell[1]; Kim Ekroos[2]; Jacob N. Marcus[1]; Smith M. Smith[1]; *[1]Merck & Co., Inc., Rahway, NJ; [2]Lipidomics Consulting Ltd., Esbo, Finland*

TP 520 **Integrated Proteomic and Transcriptomic Profiling Reveals Diversity of Hippocampal Subregions and Strata at Synaptic Resolution**; Quinn Waselenchuk[1, 2, 3]; Eva Kaulich[1]; Nicole Fürst[1]; Kristina Desch[1, 2]; Julian D. Langer[1, 2]; Erin M. Schuman[1]; *[1]Max Planck Institute for Brain Research, Frankfurt, Germany; [2]Max Planck Institute of Biophysics, Frankfurt, Germany; [3]International Max Planck Research School on Cellular Biophysics, Frankfurt, Germany*

TP 521 **Spatial proteomic characterization of single amyloid plaque in murine Alzheimer's disease brains by laser capture microdissection and mass spectrometry**; Mengqi Chu[1]; Ju Wang[1]; Yun Jiao[1]; Junmin Peng[1]; *[1]Stjude children research hospital, Memphis, TN*

TP 522 **Cholesterol ester dynamics during demyelination and remyelination**; Nishama Da Silva Mohotti[1]; Hiroko Kobayashi[1]; Jenna M. Williams[1]; Meredith D Hartley[1]; *[1]University of Kansas, Lawrence, KS*

TP 523 **Mass spectrometry approach to characterize tumour heterogeneity in glioblastoma blood-brain-barrier 3D microtissues**; Maxine Lam[1]; Joey Aw[1]; Damien Tan[2]; Tianyun Zhao[1]; Andrea Pavesi[1]; Radoslaw Sobota[2]; *[1]A*STAR, Singapore, Singapore; [2]A*STAR, Singapore, Singapore*

TP 524 **Neurogenesis-related proteomics modulation in germline histone H3.3 mutations**; Elizabeth G. Porter[1]; Francisca N De Luna Vitorino[1]; Khadija D. Wilson[2]; Yixuan Xie[1]; Peter Klein[2]; Elizabeth J. Bhoj[2]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO;*

[2]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA

TP 525 **Characterization of proteome and histone post-translational modification (PTM) changes associated with N-terminal neuroepigenetic histone mutations**; Carolina Brás Costa[1]; Francisca N. L. Vitorino[1]; Joanna K Lempiainen[1]; Elizabeth G. Porter[1]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

TP 526 **Proteomic Analysis of Synaptosomes in a Huntington's Disease Mouse Model Reveals Pathological Contributions of Calcium/Calmodulin-Dependent Protein Kinase Type II**; Joanna Bons[1]; Maria A. Sanchez[1]; Elena T. Battistoni[1]; Barbara J. Bailus[1]; Swati Naphade[1]; Ningzhe Zhang[1]; Carlos Galicia Aguirre[1]; Lei Wei[1]; Ryan Quinn[1]; Lisa M. Ellerby[1]; Birgit Schilling[1]; *[1]Buck Institute for Research on Aging, Novato, CA*

TP 527 **Phosphoproteomic characterization of the dorsal anterior cingulate cortex in Schizophrenia implicates CDK1 as a regulatory enzyme in psychiatric disease**; Andrew G. DeMarco[1]; Ryan Salisbury[1]; Kevin Xu[1]; Jordan Gilardi[1]; Akayla Lewin[1]; Lambertus Klei[1]; Robert A Sweet[1]; David A Lewis[1]; Bernie Devlin[1]; Matthew L MacDonald[1, 2]; *[1]Department of Psychiatry, University of Pittsburgh, Pittsburgh, PA; [2]Health Sciences Mass Spectrometry Core, University of Pittsburgh, Pittsburgh, PA*

TP 528 **Electrophysiology-Assisted Single-Neuron Proteomics Reveals Gender Differences in Proteome Profile in the Locus Coeruleus of the Adult Mouse**; Jingyun Lee[1]; Zhong-Min Wang[1]; María Laura Messi[1]; Carol Milligan[1]; Cristina Maria Furdui[1]; Osvaldo Delbono[1]; *[1]Wake Forest University School of Medicine, Winston-Salem, NC*

TP 529 **An optimized protocol for the preparation of protein-dextran mixtures for mass spectrometry-based proteomics analysis of microperfusates**; Xiaoli Wang[1]; M Cristine C. Charlesworth[1]; Cecile Riviere-Cazaux[1]; Benjamin J. Madden[1]; Kenneth L. Johnson[1]; Terry C. Burns[1]; Akhilesh Pandey[1]; Jun Zhong[1]; *[1]Mayo Clinic, Rochester, MN*

TP 530 **Age-dependent changes in the molecular signatures of mouse brain elucidated by multi-protease proteomic and phosphoproteomic analyses**; Rodrigo Mohallem[1]; Allison J. Schaser[1]; Uma K. Aryal[1]; *[1]Purdue University, West Lafayette, IN*

TP 531 **Unveiling the Proteome Signatures of Traumatic Brain Injury Development and Progression in Small Extracellular Vesicles**; Mojibola O Fowowe[1]; Cristian D Gutierrez-Reyes[1]; Moyinoluwa Adeniyi[1]; Sherifdeen B Onigbinde[1]; Ayobami Oluokun[1]; Firas Kobeissy[2]; Stefania Mondello[3]; Ava M Puccio[4]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA; [3]Department of Biomedical and Dental Sciences and Morphofunctional Imaging, University of Messina, Messina, Italy; [4]Department of Neurological Surgery, University of Pittsburgh, Pittsburgh, PA*

TP 532 **Optimization of isolating synaptic vesicles for comprehensive glycoproteomic and neuropeptidomic analysis in neurodevelopmental disorders**; Julia L Hoffman[1]; Thao U Duong[1]; Elliot Patrenets[2]; Hannah N Miles[3]; Ashley Phetsanthad[1]; Pamela R Westmark[4, 5]; Cara J Westmark[4, 5]; Lingjun Li[1, 3, 5]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin; [2]University of Wisconsin-Madison, Department of Integrative Biology, Madison, Wisconsin; [3]University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin; [4]University of Wisconsin-Madison, Department of Neurology, Madison, Wisconsin; [5]University of Wisconsin-Madison, Molecular Environmental Toxicology Center, Madison, Wisconsin*

TP 533 **Detection and characterization of Alzheimer's Disease biomarkers using Liquid Chromatography Ion Mobility Mass spectrometry (LC-IM-MS/MS)**; Kimberly Y. Kartowikromo[1]; Zachary E. Love[1]; Orobola E. Olajide[1]; Ahmed M. Hamid[1]; *[1]Auburn University, AUBURN, AL*

TP 534 **Analysis of Anterior Cerebral Artery and Cortex Tissue in Alzheimer's Disease**; Margaret Downs[1]; Ashley Tai[1]; Thor D. Stein[2, 3, 4]; Yanhang Zhang[5, 6, 7]; Joseph Zaia[1]; *[1]Boston University Chobanian & Avedisian School of Medicine, Boston, MA; [2]Pathology and Laboratory Medicine, Boston University, Boston, MA; [3]VA Boston Healthcare system, U.S. Department of Veteran Affairs, Jamaica Plain, MA; [4]VA Bedford Healthcare System, US Department of Veteran Affairs, Bedford, MA; [5]Department of Mechanical Engineering, Boston University, Boston, MA; [6]Department of Biomedical Engineering, Boston University, Boston, MA; [7]Division of Materials Science and Engineering, Boston University, Boston, MA*

TP 535 **Elucidating cellular and molecular features of white matter hyperintensities in Alzheimer's disease with multimodal imaging**; Claire F Scott[1]; Cody R Marshall[2, 3]; Madeline E Colley[3, 4]; Elena Solopova[5]; Lukasz Migas[6]; Angela R.S. Kruse[3, 7]; Katerina V Djambazova[3, 7]; Wilber Romero Fernandez[5]; Matthew S Schrag[5]; Raf Van De Plas[3, 6]; Jeffrey M Spraggins[2, 3, 4, 7, 8]; *[1]Vanderbilt University, Nashville, TN; [2]Chemical and Physical Biology Program, Vanderbilt University, Nashville, TN; [3]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN; [5]Department of Neurology, Vanderbilt University, Nashville, TN; [6]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [7]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [8]Department of Chemistry, Vanderbilt University, Nashville, TN*

TP 536 **Understanding the Impact of Genetic Variants on Systemic Factors in Alzheimer's Disease with Mass Spectrometry Proteogenomics**; Benjamin Lacar[1]; Amir Alavi[1]; Harendra Guturu[1]; Shadi Ferdosi[1]; Alexey Stukalov[1]; Guhan Venkataraman[1]; Matthijs De Geus[2]; Hiroko Dodge[2]; Chao-Yi Wu[2]; Pia Kivisakk[2]; Sudeshna Das[2]; Bradley Hyman[2]; Serafim Batzoglou[1]; Steven E. Arnold[2]; Asim Siddiqui[1]; *[1]Seer, Inc., Redwood City, CA; [2]Massachusetts General Hospital (MGH), Charlestown, MA*

TP 537 **Overexpression of hSOD1G37R ALS mutant within the spinal cord of mice is characterized by proteomic changes linked to microglial activation**; Lester S. Manly[1]; Anne M. Roberts[1]; Eric B. Dammer[2]; Ankit P. Jain[1]; Nicholas T. Seyfried[1, 2]; Peter J. Crouch[3]; Blaine R. Roberts[1, 2]; *[1]Department of Biochemistry, Emory University, Atlanta, GA; [2]Department of Neurology, Emory University, Atlanta, GA; [3]School of Biomedical Sciences, University of Melbourne, Melbourne, Australia*

TP 538 **Novel brain-penetrant inhibitor of G9a methylase blocks Alzheimer's disease proteopathology for precision medication**; Ling Xie[1]; Ryan Nicholas Sheehy[1]; Yan Xiong[2]; Adil Muneer[3]; Jin Jian[2]; Juan Song[1]; Xian Chen[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Icahn School of Medicine at Mount Sinai, New York, NY; [3]University of North Carolina Chapel Hill, Chapel Hill, NC*

TP 539 **Psychedelics-induced proteomic alterations within the brain**; Kacper Lukasiewicz[1]; Tomasz Kowalczyk[1]; Arkadiusz Zbikowski[1]; Napoleon Waszkiewicz[1]; Adam Kretowski[1]; Michal Ciborowski[1]; Dominik Cysewski[1]; *[1]Medical University of Bialystok, BIALYSTOK, Poland*

NUCLEIC ACIDS AND OLIGONUCLEOTIDES II
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TP 540 **Streamlined IP-RP-LCMS workflow for siRNA characterization and routine impurity profiling**; CHEN-CHUN CHEN[1]; Matt Sorensen[2]; Todd Maloney[2]; *[1]Eli Lilly and Company, Indianapolis, IN; [2]Eli Lilly & Company, Indianapolis, IN*

TP 541 **Negative Electron Transfer Collision-Induced Dissociation of G-quadruplexes: Uncovering the Guanine Radical Anion Loss Pathway**; Nicole M Brundridge[1]; Jordan M Fritz[1]; Jonathan Dickerhoff[1]; Danzhou

Yang[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

TP 542 **Rapid Oligonucleotide Separation and Sequence Confirmation Using Untargeted LC-UV-MS/MS and a New Data Analysis Software**; Katherine Sanders[1]; Amber Henry[1]; Kevin Ray[1]; *[1]Millipore Sigma, St. Louis, MO*

TP 543 **Evaluation of Novel Triplex-Binding Ligands Using Native Mass Spectrometry**; Landy Gu[1]; Nghia Tran[1]; Vanessa Marie Rangel[1]; Liang Xue[1]; *[1]University of The Pacific, Stockton, CA*

TP 544 **Investigation on Naturally Occurring Flavonoids on Their Ability to Stabilize DNA Triplexes**; Nghia T Tran[1]; Landy Gu[1]; Vanessa Rangel[2]; Tiffanie Jiang[2]; Holly Jiang[2]; Sabrina Ton[2]; Justin Shen[2]; Polina Eidelberg[2]; Liang Xue[2]; *[1]University of The Pacific, Stockton, CA; [2]University of the Pacific, Stockton, CA*

TP 545 **Proximity proteomics profiling of RNA G-quadruplex-interacting proteins in live cells**; Xiaochen Liang[1]; Feng Tang[2]; Yinsheng Wang[2]; *[1]University of California Riverside, Riverside, CA; [2]University of California, Riverside, Riverside, CA*

TP 546 **HPLC Fractionation and LCMS/MS Characterization of Human tRNA species**; Jennifer Kist[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 547 **Analysis of RNA epigenetic modifications in peripheral white blood cells by mass spectrometry**; Cheng Guo; *Zhejiang University, Hangzhou, China*

TP 548 **A mass spectrometry-based pipeline for identifying RNA modifications involved in cancer cell adaptation**; Aurore ATTINA[1]; Amandine Amalric[2]; Jérôme Vialaret[1]; Sylvain Lehmann[1]; Alexandre David[3]; Christophe Hirtz[1]; *[1]LBPC-PPC, Montpellier University, IRMB CHU Montpellier, INM INSERM, Montpellier, France; [2]IGF, INSERM, CNRS, MONTPELLIER, France; [3]Montpellier Cancer Research Institute, INSERM Montpellier, MONTPELLIER, France*

TP 549 **Evaluation of crosslinked peptide–RNA oligonucleotides by NanoLC-ESI-MS/MS to Identify the Sequence and Position of the Crosslinked RNA**; Sinem Apaydin[1]; Aleksandar Chernev[1]; Ralf Pflanz[1]; Monika Raabe[1]; Henning Urlaub[1, 2]; *[1]Bioanalytical Mass Spectrometry Group, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; [2]Bioanalytics Group, Department for Clinical Chemistry, University Medical Center Göttingen, Goettingen, Germany*

TP 550 **Characterisation of small RNA-based therapeutics by fast, sensitive, and reproducible low flow LC-MS/MS method**; Silvia Millan Martin[1]; Felipe Guapo[1]; Nora Crushell[1]; Sara Carillo[1]; Ken Cook[2]; Alexander Boris Schwahn[3]; Shanhua Lin[4]; Jonathan Bones[1, 5]; *[1]The National Institute for Bioprocessing Research & Training, Dublin, Ireland; [2]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [3]Thermo Fisher Scientific, Reinach, Switzerland; [4]Thermo Fisher Scientific, Sunnyvale, CA; [5]School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland*

TP 551 **Method considerations for therapeutic ASO RNA analysis. Adducts and insource impurity generation**; Ken Cook[1]; Ulrik Mistarz[2]; Alexander Schwahn[3]; Fiona Rupprecht[4]; *[1]Thermo Fisher Scientific, Morpeth, United Kingdom; [2]Thermo Fisher Scientific, Allerød, Denmark; [3]Thermo Fisher Scientific, Reinach, Switzerland; [4]Thermo Fisher Scientific, Bremen, Germany*

TP 552 **Characterization of oligonucleotide therapeutics on an Ultra-High Mass Range Hybrid Quadrupole-Orbitrap Mass Spectrometer**; Kristina Srzentic[1]; Robert L Ross[2]; Andrew Norris[1]; Alexander Boris Schwahn[1]; Ales Holfeld[1]; *[1]Thermo Fisher Scientific, Reinach, Switzerland; [2]Thermo Fisher Scientific, Lexington, MA*

TP 553 **A data-independent acquisition mass spectrometry workflow for characterizing mRNA therapeutics**; Hiroshi Nakayama[1]; Masami Koike[1]; Yuko Nobe[2]; Yoshiki Nagashima[3]; Daisuke Higo[3]; Masato Taoka[2]; *[1]RIKEN Center for Sustainable Resource Science, Wako, Japan; [2]Tokyo Metropolitan University, Hachioji, Japan; [3]ThermoFisher Scientific, Yokohama, Japan*

TP 554 **SynONIM: A synthetic nucleic acid and oligonucleotide impurity and modifications database to facilitate information sharing and facilitate MS data processing**; Jennifer L Lippens[1]; Biancamaria Florenzi[2]; Katyeny Manuela Da Silva[1]; Thomas Neefs[1]; Youzhong Liu[1]; Nicolas Sauwen[2]; Thomas De Vijlder[1]; *[1]Janssen Pharmaceutica NV, Beerse, Belgium; [2]Open Analytics, Antwerpen, Belgium*

TP 555 **A Fully Automated Data Workflow for Quality Monitoring of Oligonucleotide Therapeutics**; YAARUB MUSA[1]; Catherine Evans[1]; Aude Tartiere[2]; Can Cui[3]; Stephen Kok[2]; Arnd Brandenburg[1]; *[1]Genedata AG, Basel, Switzerland; [2]Genedata Inc, San Francisco, CA; [3]Genedata Inc., Lexington, Massachusetts*

TP 556 **NASEWEIS: a fast web-service for the analysis of Oligonucleotide modifications**; Samuel P Wein[1]; Oliver Kohlbacher[1]; *[1]University of Tübingen, Tübingen, Germany*

TP 557 **Alkylimidazolium labeling of oligonucleotides improves electrospray ionization efficiencies to enable characterization of ribosomal RNA in neurons**; Max Sharin[1]; Kevin D Clark[1]; *[1]Tufts University, Medford, MA*

TP 558 **Prediction of Collision-Induced Dissociation Spectra of Deprotonated Oligonucleotides**; Zhongqi Zhang[1]; Jason L. Richardson[1]; *[1]Amgen Inc., Thousand Oaks, CA*

TP 559 **Oligonucleotides characterization using single quadrupole mass spectrometer for quality control**; Udara Jayasundara[1]; Vikki Johnson[1]; Stephen Kurzyniec[1]; Evelyn Wang[2]; Yoshiyuki Okamura[2]; *[1]Shimadzu scientific instruments, Carlsbad, CA; [2]Shimadzu Scientific Instruments, Columbia, MD*

TP 560 **Computer Modeling of the Effectiveness of MS1 and MS2 for RNA Sequence Confirmation**; Clara Bern[1]; Maria Basanta-Sanchez[2]; Steven Broome[2]; Ignat Shilov[2]; Wilfred Tang[2]; Marshall W. Bern[2]; *[1]Carlmont High School, Belmont, CA; [2]Protein Metrics, LLC, Cupertino, CA*

TP 561 **Investigations in LC/MS amd LC/UV Analysis of Very Large Intact Oligonucleotides Using Various IP-RP Mobile Phases and Column Chemistries**; Sujatha Chilakala[1]; Roxana Eggleston-Rangel[1]; Michael McGinley[1]; Helen Harrington[2]; *[1]Phenomenex, Torrance, CA; [2]Phenomenex, London, United Kingdom*

TP 562 **RNA identification using Zn2+/Tris catalyzed hydrolysis and liquid chromatography-mass spectrometry**; Audriy Jebet[1, 2, 3, 4]; Raobo XU[1, 2, 3, 4]; Liqing He[1, 2, 3, 4]; Xipeng Ma[1, 2, 3, 4]; Eugene G. Mueller[1]; Craig J. McClain[1, 2, 4, 5, 6]; Xiang Zhang[1, 2, 3, 4, 6]; *[1]University of louisville, Louisville, KY; [2]University of Louisville Hepatobiology & Toxicology Center of Biomedical Research Excellence, Louisville, KY; [3]University of Louisville Alcohol Research Center, Louisville, KY; [4]Center for Regulatory and Environmental Analytical Metabolomics, Louisville, KY; [5]Department of Medicine, Louisville, KY; [6]Department of Pharmacology and Toxicology, University of Louisville, Louisville, KY*

TP 563 **Ultra-sensitive quantitation of therapeutic oligonucleotide in human plasma by a high resolution accurate mass Orbitrap mass spectrometer**; Hao Yang[1]; Min Du[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Lexington, MA*

TP 564 **Identification of HELLS as a Novel G-quadruplex Helicase**; Zi Gao[1]; Xiaomei He[1]; Yie Woon Chong[1]; Jun Yuan[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

TP 565 **A Novel and Highly Effective LC/MS Method for Phosphorodiamidate Morpholino Oligomer (PMO) Impurity and Sequencing Analysis**; Guannan Li[1]; Peter Rye[2]; Vincent Guerlavais[3]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Lexington, MA; [3]Sarepta Therapeutics, Cambridge, MA*

TP 566 **Oligonucleotide Workflow Incorporating Nuclease-Conjugated Beads with LC-MS/MS**; Shweta Chhajed[1]; William M McGee[1]; Robert Ross[1]; Voin Petrović[2]; Axl Alois Neurauter[2]; Dave Odelson[1]; James L Stephenson Jr[1];

[1]Thermo Fisher Scientific, Lexington, MA; [2]Thermo Fisher Scientific, Oslo, Norway

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TP 567 **Dia-PASEF for in-depth immunopeptidomics analysis: Challenges and new opportunities**; Kristina Marx[1]; Naomi Hoenisch Gravel[2, 3]; Juliane Walz[3, 4, 5, 6]; Pierre-Olivier Schmitt[7]; Torsten Mueller[1]; *[1]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [2]Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tuebingen, Tuebingen, Germany; [3]Cluster of Excellence iFIT (ECX2180) "Image-Guided and Functionally Instructed Tumor Therapies"; University of Tuebingen, Tuebingen, Germany; [4]Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tübingen, Tübingen, Germany; [5]Clinical Collaboration Unit Translational Immunology, Department of Internal Medicine, University Hospital Tuebingen, Tuebingen, Germany; [6]German Cancer Consortium (DKTK) and German Cancer Research Center (DKFZ), partner site Tuebingen, Tuebingen, Germany; [7]Bruker France SAS, Wissembourg, France*

TP 568 **Investigating the Impact of Copper Toxicity on Antimicrobial Peptides in Callinectes sapidus: A Mass Spectrometry Approach to Hemolymph and Hemocytes**; Tina C Dang[1]; Wenxin Wu[2]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin; [2]University of Wisconsin-Madison, Department of Chemistry, Madison, WI*

TP 569 **Alterations in Neuropeptide Distribution in Stomatogastric Nervous System of Blue Crab Callinectes sapidusUnder Hypoxia**; Thao U Duong[1]; Penghsuan Huang[1]; Ashley Phetsanthad[1]; Vu Ngoc Huong Tran[2]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [2]University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin*

TP 570 **Quantitative Assessment of Feeding-Induced Neuropeptidome Changes via Multiplexed Mass Spectrometry**; Mitchell Gray[1]; Lauren Fields[1]; Tina C Dang[2]; Angel E Ibarra[1]; Wenxin Wu[1]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin; [2]University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin*

TP 571 **Neuropeptide Secretion in Crustacean in Response to Feeding via In vivo Microdialysis**; Vu Ngoc Huong Tran[1]; Gaoyuan Lu[1]; Thao U Duong[2]; Zachary P Del Mundo[1]; Lingjun Li[1, 2]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

TP 572 **Circadian changes in the cerebrospinal fluid peptidome & proteome found by nanoLC-IMS-QqTOF**; Shannon D Berneche[1, 2]; Sarah Asif[2]; Wei-Chun Kao[2]; Taylor Jorgensen[2]; Dharmeshkumar Parmar[3]; Martha U Gillette[2, 4]; Jonathan V Sweedler[2, 3]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL; [2]Neuroscience Program, University of Illinois Urbana-Champaign, Urbana, IL; [3]Department of Chemistry, University of Illinois Urbana-Champaign, Champaign, IL; [4]Department of Cell and Developmental Biology, University of Illinois Urbana-Champaign, Urbana, IL*

TP 573 **In-silico library and two-step search improve data-independent acquisition immunopeptidomics**; Yuanliang Zhang[1]; Lei Chen[1]; Qian Zhao[1]; *[1]The Hong Kong Polytechnic University, Hong Kong, Hong Kong*

TP 574 **Advancing Clinical Peptidome Profiling in Plasma with a Robust High-Throughput Workflow**; Andreas Zellner[1]; Steffen Tiedt[2]; Chien-Yun Lee[1]; *[1]Technical University of Munich (TUM), Freising, Germany; [2]Ludwig-Maximilians-University of Munich (LMU), Munich, Germany*

TP 575 **An AI-driven, proteogenomics-based and complete workflow for novel neoantigen discovery**; Qing Zhang[1]; Kyle Hoffman[1]; Sahar Rabinoviz[1]; Chao Peng[2]; Lei Xin[1]; Baozhen Shan[1]; *[1]Bioinformatics Solutions Inc, Waterloo, ON; [2]BaizhenBio Inc., Wuhan, China*

TP 576 **Using targeted mass spectrometry to characterize the mechanism of action for a novel T cell-priming vaccine delivery system**; Richard Brase[1]; Hager Mohamed[1]; Aykan Karabudak[1]; Xiaofang Huang[1]; *[1]Emergex Vaccines, Doylestown, PA*

TP 577 **Streamlined LC/MS methods to quantitate MHC-I peptides in the development of neoantigen-directed therapeutics**; Arun Tailor[1]; Jason LaMar[1]; Alisa Arata[1]; Sebastian Guelman[1]; Surinder Kaur[1]; Ola M Saad[1]; *[1]Department of BioAnalytical Sciences, Genentech, Inc., South San Francisco, California*

TP 578 **Total HLA Class II Quantification in Dendritic Cells (DCs) to Compliment MHC Associated Peptide Proteomics (MAPPs) for Immunogenicity Risk Assessment**; Jason LaMar[1]; Alisa Arata[2]; Violet Lee[2]; Arun Tailor[2]; Sylvia Wong[2]; Surinder Kaur[2]; Ola M Saad[2]; *[1]Genentech - South San Francisco, CA, South San Francisco, CA; [2]Genentech Inc, South San Francisco, CA*

TP 579 **Maximizing immunopeptide identification and reproducibility from minute pediatric solid tumor biopsy samples**; Peiyao Li[1]; Richa Kapoor[1]; John M. Maris[1, 2]; Diego Assis[3]; Matthew Willetts[3]; Hossein Fazelinia[1]; Lynn A Spruce[1]; *[1]Children's Hospital of Philadelphia, Philadelphia, PA; [2]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; [3]Bruker Scientific, LLC, Billerica, MA*

TP 580 **ImmunoResource: Noncanonical MHC-I associated peptide database compounded by proteogenomic analysis of immunopeptidome data**; Yoonwoo Lee[1]; Seunghyuk Choi[2]; Eunok Paik[1, 2]; *[1]Department of Artificial Intelligence, Hanyang University, Seoul, South Korea; [2]Department of Computer Science, Hanyang University, Seoul, South Korea*

TP 581 **Towards a comprehensive panMHC-II MAPPs (MHC-II Associated Peptide Proteomics) analysis to assess immunogenicity risks of biotherapeutics**; Axel Ducret[1]; Maureen Bardet[1]; Shahrzad Tavalei[1]; Katharina Hartman[1]; Céline Marban-Doran[1]; *[1]Roche Innovation Center Basel (RICB), Switzerland, Switzerland*

TP 582 **Development of a novel high-sensitivity peptidomics platform based on capillary electrophoresis coupled with a high-resolution mass spectrometry**; Tomoaki Nitta[1]; Kazunori Sasaki[1]; Hiroyuki Yamamoto[1]; Kenjiro Kami[1]; *[1]Human Metabolome Technologies, Inc., Tsuruoka, Japan*

TP 583 **TIMSrescore: timsTOF-optimized PSM rescoring boosts identification rates for immunopeptidomics**; Arthur Declercq[1]; Jonathan Krieger[2]; George Rosenberger[3]; Ralf Gabriels[1]; Robbin Bouwmeester[1]; Tharan Srikumar[2]; Sven Degroeve[1]; Dennis Trede[4]; Lennart Martens[1]; *[1]VIB-UGent Center for Medical Biotechnology, Gent, Belgium; [2]Bruker Ltd., Milton, ON; [3]Bruker Switzerland AG, Faellanden, Switzerland; [4]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

TP 584 **Abemaciclib differentially affects the immunopeptidome of breast cancer subtypes**; Robin Minati[1, 2]; Eralda Kina[1, 2]; Eric Bonneil[1]; Joel Lanoix[1]; Marie-Pierre Hardy[1]; Krystel Vincent[1]; Claude Perreault[1, 3]; Pierre Thibault[1, 4]; *[1]Institute of Research in Immunology and Cancer, Université de Montréal, Montreal, QC; [2]Molecular biology program, Université de Montréal, Montréal, QC; [3]Department of Medicine, Université de Montréal, Montreal, QC; [4]Department of Chemistry, Université de Montréal, Montréal, QC*

TP 585 **Distinguishing MIPs in the cell surface or in processing by MS with immunoprecipitation and Mild Acid Elution methods**; Chao Peng[1]; Ping Wu[1]; Haofei Miao[1]; Ling Li[1]; Baozhen Shan[1]; *[1]BaizhenBio Inc., Wuhan, China*

TP 586 **Advanced Immunopeptidomics Pipeline Unveils Significantly Expanded Noncanonical Neoantigen Repertoire Following Spliceosome Perturbation**;

Jongmin Choi[1]; Seunghyuk Choi[1]; Elizabeth A. Bowling[1]; Matthew V. Holt[1]; Kristen L. Karlin[1]; Matthew Willetts[2]; Ruben Shrestha[2]; Diego Assis[2]; Jarey H. Wang[1]; Sara J. Wright[1]; Adithya Balasubramanian[1]; Hyun-Sung Lee[1]; Thomas Westbrook[1]; Bing Zhang[1]; [1]*Baylor College of Medicine, Houston, TX;* [2]*Bruker life sciences, Billerica, MA*

TP 587 **No enzyme? No problem! An accessible, scalable multi-omic cloud-based solution for efficient MS-based endogenous peptidomics and immunopeptidomics**; Reid Wagner[1, 2]; James E Johnson[1, 2]; Subina Mehta[1]; Kyle Richards[1]; Suzanne Coleman[1]; David A Largaespada[1]; Monica E Kruk[1]; Chris H Wendt[1, 3]; Bing Zhang[4]; Fengchao Yu[5]; Alexey I Nesvizhskii[5]; Pratik D. Jagtap[1]; Tim Griffin[1]; [1]*University of Minnesota, Minneapolis, MN;* [2]*Minnesota Supercomputing Institute, Minneapolis, MN;* [3]*Minneapolis VA Health Care System, Minneapolis, MN;* [4]*Baylor College of Medicine, Houston, Texas;* [5]*University of Michigan, Ann Arbor, Michigan*

TP 588 **Trapped ion mobility-coupled mass spectrometry reveals high frequent tumor-associated antigens in chronic lymphocytic leukemia**; Naomi Hoenisch Gravel[1, 2]; Jonas Scheid[1, 2, 3]; Marcel Wacker[1, 2]; Yacine Maringer[1, 2]; Jens Bauer[1, 2]; Juliane Walz[1, 2, 4, 5]; [1]*Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tuebingen, Tuebingen, Germany;* [2]*Cluster of Excellence iFIT (EXC2180) "Image-Guided and Functionally Instructed Tumor Therapies"; University of Tuebingen, Tübingen, Germany;* [3]*Quantitative Biology Center QBIC), University of Tübingen, Tübingen, Germany, Tübingen, Germany;* [4]*Clinical Collaboration Unit Translational Immunology, Department of Internal Medicine, University Hospital Tuebingen, Tuebingen, Germany;* [5]*German Cancer Consortium (DKTK) and German Cancer Research Center (DKFZ), partner site Tuebingen, Tuebingen, Germany*

TP 589 **Advancing Low input Chromatography: Developing a novel Column for Improved Immunopeptidomics IDs**; Benoit Fatou[1]; Michael Krawitzky[2, 3]; Ruben Shrestha[4]; Diego Assis[5]; Nicholas Cheung[6]; Darshit Shah[6]; Robert Salzler[6]; Matthew Willetts[7]; [1]*Bruker Scientific, LLC, Billerica, MA;* [2]*Bruker Daltonics, San Jose, CA;* [3]*Bruker Switzerland AG, Faellanden, Switzerland;* [4]*Bruker Scientific LLC, San Jose, CA;* [5]*Bruker Scientific, Billerica, MA;* [6]*Regeneron Pharmaceuticals, Tarrytown, NY;* [7]*Bruker Daltonics GmbH & Co. KG, Billerica, MA*

TP 590 **Assessing a Single Mutation's Effect on Immunogenicity of FLT3L-Fc**; Qui Phung[1]; Yinyin Li[1]; Zhenru Zhou[1]; Sivan Cohen[1]; Travis Bainbridge[1]; Mercedesz Balazs[1]; Jennie Lill[1]; Dan Qin[1]; [1]*Genentech Inc, South San Francisco, CA*

TP 591 **Mhcquant enables scalable and reproducible immunopeptidomics analyses with enhanced peptide identification using streamlined peptide property predictors**; Jonas Scheid[1, 2, 3]; Steffen Lemke[1, 2, 3]; Naomi Hoenisch Gravel[1, 2]; Timo Sachsenberg[4, 5]; Arthur Declercq[6, 7]; Ralf Gabriels[6, 7]; Jens Bauer[1, 2]; Leon Bichmann[8]; Marissa Lisa Dubbelaar[1, 2, 3]; Juliane Sarah Walz[1, 2, 9, 10]; Sven Nahnsen[3, 11]; [1]*Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tübingen, Tübingen, Germany;* [2]*Cluster of Excellence iFIT (EXC2180) "Image-Guided and Functionally Instructed Tumor Therapies", University of Tübingen, Tübingen, Germany;* [3]*Quantitative Biology Center (QBiC), University of Tübingen, Tübingen, Germany;* [4]*Institute for Bioinformatics and Medical Informatics, University of Tubingen, Tubingen, Germany;* [5]*Applied Bioinformatics, Department of Computer Science, University of Tübingen, Tübingen, Germany;* [6]*VIB-UGent Center for Medical Biotechnology, VIB, Ghent, Belgium;* [7]*Department of Biomolecular Medicine, Ghent University, Ghent, Belgium;* [8]*Center for Systems and Engineering Immunology (CSEI), School of Medicine, Yale University, New Haven, CT;* [9]*Clinical Collaboration Unit Translational Immunology, Department of Internal Medicine, University Hospital Tuebingen, Tuebingen, Germany;* [10]*German Cancer Consortium (DKTK) and German Cancer Research Center (DKFZ), partner site Tuebingen, Tuebingen, Germany;* [11]*Department for Computer Science, Biomedical Data Science, University of Tübingen, Tübingen, Germany*

TP 592 **Discovering physiological substrates for the coronavirus host receptor protease ACE2 using stable isotope signature labeling**; Fabian Schulte[1]; Markus Hardt[1]; [1]*Forsyth Institute, Cambridge, MA*

TP 593 **Thunder-DDA-PASEF boosted by MS2Rescore enables high sensitivity and high-coverage immunopeptidomics**; David Gomez-Zepeda[1, 2]; Danielle Arnold-Schild[3]; Julian Beyrle[1, 2]; Arthur Declercq[4, 5]; Ralf Gabriels[4, 5]; Annica Preikschat[3]; Mateusz Lacki[3]; Aurélie Hirschler[6]; Jeewan Babu Rial[6]; Christine Carapito[6]; Lennart Martens[4, 5]; Ute Distler[3]; Hansjörg Schild[3]; Stefan Tenzer[1, 2, 3]; [1]*Helmholtz Institute for Translational Oncology Mainz (HI-TRON Mainz) – A Helmholtz Institute of the DKFZ, Mainz, Germany;* [2]*DKFZ German Cancer Research Center, Heidelberg, Germany;* [3]*University Medical Center Mainz, Mainz, Germany;* [4]*VIB - UGent Center for Medical Biotechnology, Gent, Belgium;* [5]*Department of Biomolecular Medicine, Ghent University, Ghent, Belgium;* [6]*BioOrganic Mass Spectrometry Laboratory (LSMBO), IPHC UMR 7178, University of Strasbourg, CNRS, ProFI, Strasbourg, France*

TP 594 **A Semi-Targeted Orbitrap Tribrid Method for Simultaneous Quantification and Discovery of Immunopeptides**; David Bergen[1]; Lilian R Heil[1]; Jingjing Huang[1]; Tonya Pekar Hart[1]; Rafael Melani[1]; Vlad Zabrouskov[1]; [1]*Thermo Fisher Scientific, San Jose, CA*

TP 595 **Immunopeptidomic landscape of non-small cell lung carcinoma**; Kiran K. Mangalaparthi[1]; Partho S. Sen[1]; Richard K. Kandasamy[1]; Aaron S. Mansfield[2]; Akhilesh Pandey[1, 3]; [1]*Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, MN 55905;* [2]*Department of Oncology, Mayo Clinic, Rochester, MN 55905;* [3]*Center for Individualized Medicine, Mayo Clinic, Rochester, MN 55905*

TP 596 **Predicting effectively complete immunopeptidome spectral libraries to improve the detection of neoantigens**; Lewis Geer[1]; Douglas Slotta[1]; [1]*NIST, Gaithersburg, MD*

PHOSPHOPEPTIDES AND PHOSPHOPROTEINS
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TP 597 **Proteomics and Phosphoproteomics Reveals Unique Alterations in KRASand P53Mutant Colorectal Cancer Spheroids after Fatty Acid Synthase Inhibition**; Brian D Fries[1]; Amanda B Hummon[1, 2]; [1]*The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH;* [2]*Comprehensive Cancer Center, Columbus, OH*

TP 598 **Towards high-dimensional phosphoproteomics with data-independent acquisition and μPhos**; Denys Oliinyk[1]; Ilka Klose[1]; Dilfuza Ernafasova[1]; Felix Schneidmadel[1]; Florian Meier[1]; [1]*University Klinikum Jena, Jena, Germany*

TP 599 **Phosphoproteomic analysis of low-input FFPE tissue samples with DIA-MS method**; Stephanie Zalesak-Kravec[1]; Yeoun Jin Kim[1]; David J Clark[1]; [1]*AstraZeneca, Gaithersburg, MD*

TP 600 **Systematic optimization of automated phosphopeptide enrichment for high-sensitivity phosphoproteomics**; Patricia Bortel[1]; Ilaria Piga[2]; Claire Koenig[2]; Christopher Gerner[1]; Ana Martinez-Val[2, 3]; Jesper Velgaard Olsen[2]; [1]*Department of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria;* [2]*Novo Nordisk Foundation Center for Protein Research, Proteomics Program, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark;* [3]*Centro Nacional de Investigaciones Cardiovasculares Carlos III (CNIC), Madrid, Spain*

TP 601 **High throughput semi-automated platform for the identification of post-translational modifications (PTMs) specific biomarkers from plasma samples**; Santosh D. Bhosale[1]; Angel Keoseyan[1]; Josselin Ortiz[1]; Nathan Hendricks[1]; Annie Moradian[1]; Susan M. Mockus[1]; [1]*Precision*

Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA

TP 602 **Dissecting the Temporal Dephosphorylation of DNA Damage Response Proteins by SPN-PP1 using DIA Phospho-proteomics**; Mi Young Son[1]; Minkyu Kim[1]; *[1]UT Health Science Center at San Antonio, San Antonio, TX*

TP 603 **IMAC-enabled Phosphoproteomic Analysis of pLRRK2, pRab10 and pRab12 in Mouse Tissues**; Junpeng Xiao[1]; Caitlyn Keck[1]; David B Shaw[1]; Nil Tandogan-Grey[1]; Paresh Sanghani[1]; Theresa A Day[1]; Michael Chalmers[1]; *[1]Eli Lilly & Company, Indianapolis, IN*

TP 604 **Development of mass spectrometry-based methods to identify C-terminal tail residues in the Glucagon receptor that are phosphorylated following agonism**; Ian Michael Lamb[1]; Alex D White[1]; Francis S Willard[1]; Michael J Chalmers[1]; Junpeng Xiao[1]; *[1]Eli Lilly & Company, Indianapolis, IN*

TP 605 **SmartPhos: Streamlining High-Throughput, Low-input Phosphoproteomics for Dynamic Cellular Insights**; Barbara Helm[1, 2]; Dario Frey[1, 2]; Cong Quan Ta[1]; Yueyang Xie[1]; Shubham Agrawal[3]; Marcel Schilling[1]; Junyan Lu[3]; Ursula Klingmüller[1, 2]; *[1]Division Systems Biology of Signal Transduction, German Cancer Research Center (DKFZ), Heidelberg, Germany; [2]German Center for Lung Research (DZL) and Translational Lung Research Center Heidelberg (TRLC), Heidelberg, Germany; [3]Computational Omics and Precision Oncology, Heidelberg University, Faculty of Medicine, Heidelberg University Hospital, Heidelberg, Germany*

TP 606 **Quantitative Global Proteome and Phosphoproteome Analysis of Caenorhabditis elegans Embryos Utilizing a FAIMS-based DIA Platform.**; Colt D Capan[1]; Michael P Vincent[1]; Jason Copper[1]; Ibukunoluwa Sodiya[1]; Nick Burton[1]; Ryan D Sheldon[1]; Hyoungjoo Lee[1]; *[1]Van Andel Institute, Grand Rapids, MI*

TP 607 **Advancing qualitative phosphoproteomics via the integration of FAIMS and non-FAIMS analysis**; Byoung-Kyu Cho[1]; Young Ah Goo[1]; *[1]Washington University in St. Louis, St. Louis, MO*

TP 608 **SARS-CoV-2 Virion Proteomics Revealed Protein Phosphatase-1**; Jyothirmai Simhadri[1]; Philipp A Ilinykh[2, 3]; Kai Huang[2, 3]; Andrey Ivanov[1]; Xionghao Lin[1]; Tatiana Ammosova[1, 4]; Alexander Bukreyev[2, 3]; Sergei Nekhai[1, 4]; *[1]Center for Sickle Cell Disease, Howard University, Washington, DC; [2]Department of Pathology, University of Texas Medical Branch, Galveston, TX; [3]Galveston National Laboratory, Galveston, TX; [4]Department of Medicine, College of Medicine, Howard University, Washington, DC*

TP 609 **Chemoproteomic mapping of aldehyde-containing metabolite interactome by mass spectrometry**; Juhee Park[1, 2]; Jong-Seo Kim[1, 2]; *[1]School of Biological Sciences, Seoul National University, Seoul, South Korea; [2]Center for RNA Research, Institute of Basic Science (IBS), Seoul, South Korea*

TP 610 **Comprehensive phosphoproteomic analysis using integrated IMAC and antibody-based phosphopeptide enrichment and mass spectrometry**; Liyuan Jiao[1]; T. Mamie Lih[1]; Lijun Chen[1]; Yuefan Wang[1]; Jongmin Woo[1]; Hui Zhang[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

TP 611 **Classification of mass spectrometry-identified phosphosites unravels potential new functions of the unannotated phosphoproteome**; Pedro R. Cutillas; *Queen Mary University of London, London, United Kingdom*

TP 612 **A fine-tune optimization of phosphoproteomics DIA analysis for a more robust and insightful candidate selection**; Sara Ceccacci[1]; Cerina Chhuon[1]; Kevin Roger[1]; Ines Metatla[1]; Joanna Lipecka[1]; Chiara Guerrera[1]; *[1]Necker Proteomics Platform, INSERM US24, Paris, France*

TP 613 **Evaluation of phosphopeptide enrichment using different metal ions for sensitive nano-scale phosphoproteomics**; Hyeyoon Kim[1]; Marina A Gritsenko[2]; Vanessa Paurus[2]; Reta Birhanu Kitata[2]; Ronald J. Moore[2]; Rosalie K. Chu[3]; Karl K. Weitz[2]; Tao Liu[2]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Pacific Northwest National Lab, Richland, WA*

TP 614 **Top-down characterization of genetically encoded Bcl-XL phosphorylation and phosphomimetics using electron capture dissociation**; Rachel Franklin[1]; Cat Hoang Vesely[2]; Richard B. Cooley[2]; Joseph Meeuswen[1]; *[1]Agilent Technologies, Corvallis, Oregon; [2]Oregon State University- GCE4ALL Center, Corvallis, Oregon*

TP 615 **Phospho-signaling regulatory mechanisms driving beta cell insulin secretion**; Mohammad Ovais Azizzanjani[1]; Rachel Elizabeth Turn[1]; Anushweta Asthana[1]; Artemis Xu[1]; Peter K. Jackson[1]; *[1]Jackson Laboratory, Baxter Laboratory for Stem Cell Biology, Department of Microbiology & Immunology, Stanford University School of Medicine, Stanford, CA*

TP 616 **RUPE-phospho：Rapid ultrasound-assisted peptide-identification-enhanced phosphoproteomics workflowfor microscale samples**; Dongxue Wang; *Beijing Proteome Research Center, National Center for Protein Sciences, Beijing, China; The π-HuB Project Infrastructure, Guangzhou, China; International Institiute for Phronesis Medicine, Guangzhou, China; South China Institute of Biomedicine, Guangzhou, China*

TP 617 **Benchmarking Orbitrap Fusion Lumos TMT quantitation versus Orbitrap Astral LFQ data independent acquisition (DIA) mass spectrometry for phosphoproteome analysis**; Gregory K Potts[1]; Shaun McLoughlin[2]; Janice Y Lee[2]; Hua Tang[2]; Jon D Williams[2]; Scott E Warder[2]; *[1]AbbVie, Inc., North Chicago, IL; [2]AbbVie Inc., North Chicago, IL*

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TP 618 **Characterisation of stress response at the proteome and transcriptome level in rice under a range of abiotic stress conditions**; Fatemeh Habibpourmehraban[1]; Zahra Ghorbanzadeh[2]; Farhad Masoomi-Aladizgeh[1]; Yunqi Wu[1]; Sara Hamzelou[1]; Dylan Multari[1]; Ardeshir Amirkhani[1]; Mehdi Mirzaei[1]; Ghasem Hosseini Salekdeh[1]; Mohammad Reza Ghaffari[2]; Brian J. Atwell[1]; Paul A. Haynes[1]; *[1]Macquarie University, North Ryde, Australia; [2]Department of Systems Biology, Agricultural Biotechnology Research Institute of Iran (ABRII), Karaj, Iran*

TP 619 **Identification of Compounds Present in the Endangered Plant Ziziphus celata: Both Host and Endophyte Origins**; Kate Calvin[1]; Kim Pham[1]; Esmeralda Morales[1]; Jesus Hernandez[1]; *[1]South Florida State College, Avon Park, FL*

TP 620 **SPATIAL EXOMETABOLOMICS OF THE POPLAR RHIZOSPHERE GROWN IN MICROFLUIDIC SOIL-LIKE HABITATS**; Kevin J Zemaitis[1]; Jayde Aufrecht[1]; Daisy Herrera[1]; Petrus Zwart[2]; Tanya Winkler[1]; Christopher Anderton[1]; Sharon Doty[3]; Amir Ahkami[1]; Dušan Veličković[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Lawrence Berkeley National Laboratory, Berkeley, CA; [3]University of Washington, Seattle, WA*

TP 621 **Mass Spectrometry-based Methods for Selective Detection of Inositol Poly- and Pyrophosphates: Implications for Cellular Processes and Biological Significance**; Hector Najera-Gonzalez[1]; Luis Herrera-Estrella[1]; *[1]Texas Tech University, Lubbock, Texas*

TP 622 **Large scale plant protein turnover measurement: a 15N metabolic approach in development**; Will V. BIENVENUT[1]; Marie-Helene Andrieux[2]; Oliver LANGELLA[1]; Thierry Balliau[1]; Sophie COLOMBIE[2]; Mélisande BLEIN-NICOLAS[1]; *[1]GQE - le moulon, Gif sur Yvette, France; [2]Biologie du Fruit, INRAE, Bordeaux, France*

TP 623 **Widely targeted metabolomics and subsequent label-feeding analysis identified candidate metabolites that control hypocotyl elongation in the model plant Arabidopsis thaliana**; HIROMITSU TABETA[1]; Tetsuya Mori[1]; Ali Ferjani[2]; Masami Hirai[1]; *[1]RIKEN CSRS, Yokohama, Japan; [2]Tokyo Gakugei University, Koganei-shi, Japan*

TP 624 **Preliminary Identification of Specialized Metabolite Secretions and Secretory Pathways in Medicago truncatula Border Cells**; Clayton Kranawetter[1, 2, 3, 4]; Lloyd W. Sumner[1, 2, 3, 4]; [1]*University of Missouri-Columbia, Columbia, MO;* [2]*MU Metabolomics Center, Columbia, MO;* [3]*Christoper S. Bond Life Sciences Center, Columbia, MO;* [4]*Interdisciplinary Plant Group, Columbia, MO*

TP 625 **Distribution analysis of related substances to elucidate the function of phytoalexins in plant-pathogen interactions**; Kaoru Nakagawa[1]; Koji Okuda[1]; Eriko Betsuyaku[2]; Toshiya Matsubara[3]; Shigeyuki Betsuyaku[2]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*Ryukoku University, Otsu, Japan;* [3]*Shimadzu Scientific Instruments, Columbia, MD*

TP 626 **Selective precursor ion LC-MS/MS analysis of glucosinolates from food/nutraceuticals vegetal species**; Alberto Asteggiano[1]; Alex Affricano[2]; Enrica Mecarelli[1]; Federica Dal Bello[2]; Claudio Medana[2]; [1]*University of Turin, Torino, Italy;* [2]*University of Turin, Torino, Italy*

TP 627 **Integration of Omic Analyses Reveals Important Biomolecular Pathways in Photosynthetic Systems**; Mary S Lipton[1]; Kim K Hixson[1]; Carrie D Nicora[1]; Samuel O Purvine[1]; Kent J Bloodsworth[1]; Vanessa L Paurus[1]; Tanya E Winkler[1]; Nathalie Munoz[1]; [1]*Pacific Northwest National Laboratory, Richland, WA*

TP 628 **Molecular Networking Reveals Diversity of Phytohormones within a Physalis Diversity Panel**; Jennifer Shipp[1]; Daniel Ence[1]; Joe Rokicki[1]; Andrew Katz[1]; [1]*Enveda Biosciences, Boulder, CO*

TP 629 **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[1]; Bryson C. Gibbons[1]; Rosalie K. Chu[1]; James J. Moran[1]; Ljiljana Pasa Tolic[1]; Amir H. Ahkami[1]; Jennifer E. Kyle[1]; Tao Liu[1]; Mary S Lipton[1]; [1]*Battelle Pacific Northwest National Laboratories, Richland, WA*

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TP 630 **Advancing the functional and structural characterization of deamidated proteoforms by novel mass spectrometry-based strategies**; Steffen Lippold[1]; Tilman Schlothauer[2]; Feng Yang[1]; [1]*Genentech, Inc., South San Francisco, CA;* [2]*Roche Diagnostics GmbH, Penzberg, Germany*

TP 631 **Capturing TCR and peptide-HLA Interactions using Cross-linking Mass Spectrometry**; Thomas J Powell[1]; Vijaykumar Karuppiah[1]; Keir Barnbrook[1]; Martin Ebner[1]; Andrew J Creese[1]; [1]*Immunocore, Abingdon, United Kingdom*

TP 632 **O-glycosylation characterization of rhTPO based on EAD mass spectrometry**; Lingsheng Chen[1]; Hexing Song[1]; Xiang Li[2]; Ji Luo[3]; Hongxu Chen[1]; Lihai Guo[1]; [1]*SCIEX, Beijing, China;* [2]*NIFDC, Beijing, China;* [3]*SCIEX, Shanghai, China*

TP 633 **The ZenoTOF 7600 system facilitates precise determination of intact mass and identification of sequence variations in Defibrase**; Longlong Hu[1]; Ji Luo[1]; Hongxu Chen[2]; Lihai Guo[2]; [1]*SCIEX, Shanghai, China;* [2]*SCIEX, Beijing, China*

TP 634 **Structural Analysis of Monoclonal Antibody Aggregation in Dynamic Heterogeneous Systems Using Liquid Chromatography Coupled with Flash Oxidation (LC-Fox) System**; Zhi Cheng[1]; Joshua S Sharp[1, 2]; Emily Chea[1]; Scot Weinberger[1]; [1]*GenNext Technologies, Half Moon Bay, CA;* [2]*UNIVERSITY OF Mississippi, Oxford, MS*

TP 635 **Utilizing Click Chemistry for Advanced Analysis of Antibody Oxidation Intermediates using High-Resolution Intact Mass Spectrometry**; Yu Zhou[1]; Jakub Baudys[1]; John R Barr[1]; Dongxia Wang[1]; [1]*Centers for Disease Control and Prevention, Atlanta, GA*

TP 636 **Exploring structural changes of antibody-drug conjugates (ADCs) under stress by native limited proteolysis**; Xinhao Shao[1]; Nhat Le[1]; Shiyue Zhou[1]; Qunying Zhang[1]; Julie Heflin[1]; [1]*Biologics Analytical R&D – LC/ABC, Biologics CMC Development, Development Sciences, AbbVie Inc., North Chicago, Illinois*

TP 637 **Mass spectrometry based approaches designed to ensure correct chain assembly of bispecific antibodies**; Vesela Encheva-Yokoya[1]; Bodhisattwa Saha[1]; Ayesha Ali[1]; Francesca Ferlenghi[1]; Karina Bora[1]; James Graham[1]; Benedict Dirnberger[1]; [1]*Lonza, London, United Kingdom*

TP 638 **Multi-level characterization and proteoform profiling of an intact monoclonal antibody using the ZenoTOF 7600**; Sarah Nguyen[1, 2, 3]; Armelle Martelet[3]; Séverine Clavier[3]; Sarah Cianférani[1, 2]; Oscar Hernandez-Alba[1, 2]; [1]*LSMBO (University of Strasbourg), Strasbourg, France;* [2]*Infrastructure Nationale de Protéomique ProFI – FR2048, Strasbourg, France;* [3]*Sanofi R&D, Vitry-sur-Seine, France*

TP 639 **Implementation of Mass Photometry as A Novel, Single Molecule Heightened Characterization Technique for Analysis of Diverse Biotherapeutic Modalities**; Lauren F Barnes[1]; Leah Wang[1]; Mingyue Li[2]; Vicky Lin[2]; Saurabh Singh[1]; Sutapa Barua[2]; Caitlin Wappelhorst[1]; Erika Jensen[1]; Clifford Entrican[2]; Daniel Ryan[1]; Qin Zou[1]; Anne Kim[2]; Jason Rouse[2]; [1]*Pfizer Inc., Chesterfield, MO;* [2]*Pfizer Inc., Andover, MA*

TP 640 **Analytical Challenges in the Characterization of a Complex Fc Fusion Protein**; Felix Vega[1]; Eliza Dulalia[1]; Jorge Monteon[1]; Mary Nguyen[1]; [1]*Alector, South San Francisco, CA*

TP 641 **Uncovering a novel seryl-like modification on a Histidine residue of a CHO-produced mAb**; Malgorzata Szyjka[1]; Ruiyi Dong[1]; Tom Cameron[1]; Mia Rushe[1]; Joseph Amatucci[1]; Heather Cooke[1]; Jana Dolnikova[1]; You Li[1]; Xiaofeng Yang[1]; [1]*Biogen, Biologics Drug Discovery, Cambridge, MA*

TP 642 **Characterization of antibody therapeutics in early discovery**; Yuntao Zhang[1]; Aarti Jashnani[1]; Srikanth Kotapati[1]; [1]*Bristol Myers Squibb, Redwood City, CA*

TP 643 **Unveiling the Complexity of a Heavily Glycosylated Reagent Protein through Charge Detection Mass Spectrometry and other Biophysical Techniques**; Tian Tian[1]; Zoltan Szabo[2]; Nithya Srinivasan[3]; Dhan Bagal[1]; Iain D.G. Campuzano[3]; [1]*Amgen, South San Francisco, CA;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*Amgen, Thousand Oaks, CA*

TP 644 **Therapeutic Protein Charge Variant Characterization with Intact Mass and Peptide Mapping Following Microgram Preparative Capillary Isoelectric Focusing Electrophoresis Fractionation**; Thomas Menneteau[1]; Claire Butré[1]; Géry Van Vyncht[1]; Arnaud Delobel[1]; Marion Galaup[2]; Kristell Lebozec[2]; Laurence Talbot[3]; Kefei Wang[4]; [1]*Quality Assistance, Thuin, Belgium;* [2]*Acticor Biotech, Paris, France;* [3]*Bio-Techne, Noyal Châtillon sur Seiche, France;* [4]*Bio-Techne, San Jose, CA*

TP 645 **Determination of the alpha-glucosidase anti-drug antibodies epitopes in Pompe disease patient plasma samples**; Evgeniy V. Petrotchenko[1]; Andreas Hahn[2]; Christoph H. Borchers[1, 3, 4, 5]; [1]*Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC;* [2]*Department of Pediatric Neurology, University of Giessen, Giessen, Germany;* [3]*Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC;* [4]*Division of Experimental Medicine, McGill University, Montreal, QC;* [5]*Department of Pathology, McGill University, Montreal, QC*

TP 646 **In-depth O-glycosylation characterization of APOE from different expression systems ——Insights for host cell selection and drug design**; Jiang Biyun[1]; Moyin Zhou[1]; Longyun Guo[1]; Tongdan Wang[1]; Jincui Huang[1]; [1]*Wuxi Biologics(Shanghai) Co., Ltd., Shanghai, China*

TP 647 **Charge Variant Analysis of IgGs Directly from Cell Culture Supernatant using Microfluidic CE-ESI-MS**; J. Scott Mellors[1]; Adi Kulkarni[2]; Stephanie R. Klaubert[2]; Kate Yu[2]; Erin A. Redman[1]; [1]*908 Devices Inc., Morrisville, NC;* [2]*908 Devices Inc., Boston, MA*

TP 648 **Ion mobility-mass spectrometry and collision induced unfolding methods reveal structural differences in**

stressed biosimilar therapeutic products; Nicole A Rivera-Fuentes[1]; Matthew Vallano[1]; Alyssa Erlenbeck[1]; Michael R. Armbruster[1]; Amanda Cicali[1]; Youngseo Na[2, 3]; Ting Zhao[2, 4]; Mingeun Kim[4]; Anna Schwendeman[4]; Brandon T Ruotolo[1]; *[1]University of Michigan Department of Chemistry, Ann Arbor, MI; [2]University of Michigan, Ann Arbor, Michigan; [3]Department of Medicinal Chemistry, University of Michigan, Ann Arbor, MI; [4]Department of Pharmaceutical Sciences, University of Michigan, Ann Arbor, MI*

TP 649 **A Data Processing Workflow Combining Orthogonal MS/MS Fragmentation Data for Comprehensive Middle-down Analysis**; Can Cui[1]; Aude Tartiere[2]; Catherine Evans[3]; Stephen Kok[2]; Yaarub Musa[3]; Arnd Brandenburg[3]; *[1]Genedata Inc., Boston, MA; [2]Genedata Inc, San Francisco, CA; [3]Genedata AG, Basel, Switzerland*

TP 650 **Charge Variant Mass spectrometry for Analysis of biotherapeutics with Orthogonal and Fractionated sampling**; St John Skilton[1]; Xiaojing Shen[2]; Krisztina Radi[1]; Baburaj Kunnummal[2]; Kefei Wang[2]; *[1]Protein Metrics, LLC, Cupertino, CA; [2]Bio-techne Ltd., San Jose, CA*

TP 651 **Optimized native conditions for charge variant analysis using a microfluidic CE-MS platform yield higher quality data for lower titer samples**; Hampus Engstroem[1]; Erin A. Redman[2]; J. Will Thompson[2]; Adi Kulkarni[1]; Kate Yu[1]; Scott Mellors[2]; *[1]908 Devices Inc., Boston, MA; [2]908 Devices Inc., Morrisville, NC*

TP 652 **A Novel Approach to Peptide Mapping of AAV Capsid protein and Host-Cell Protein Impurities**; Sergei Saveliev[1]; Alba Katiria González Rivera[2]; Marjeta Urh[2]; Mike Rosenblatt[2]; *[1]Promega Corporation, Madison, WI; [2]Promega Corporation, Madison, Wisconsin*

TP 653 **Automated Workflow Improvements for Minimizing Artificial Deamination in Peptide Mapping of Therapeutic Monoclonal Antibodies and ADCs**; Yilin Han[1]; Teresa Schu[1]; Yuanhui Ma[1]; Daniela Olszova[1]; Tawnya Flick[1]; Simon Letarte[1]; *[1]Gilead Sciences, Oceanside, CA*

TP 654 **Utalization of Intact Reconstruction to Characterize Bi-specific antibodies**; William Resager[1]; Nancy Fernandes[2]; *[1]Protein Metrics, Ridgefield, WA; [2]Lonza Biologics, Portsmouth, New Hampshire*

TP 655 **Flash Characterization of mAbs using a Combination of Reagents via Automated On-Line Microdroplet Reaction**; Michael D Knierman[1]; Hui Zhao[2]; Jim Lau[2]; *[1]Agilent, Indianapolis, IN; [2]Agilent Technologies, Wilmington, DE*

TP 656 **Characterization of a Novel Disulfide Rich Therapeutic Antibody Fragment and determination of its SARS-Cov-2 RBD Binding Epitope by Mass Spectrometry**; Michael Bacica[1]; Christopher Warner[2]; *[1]Primrose Bio, Inc., San Diego, CA; [2]Primrose Bio, Inc., San Diego, California*

TP 657 **Conformational Heterogeneity of the Monoclonal Antibody NISTmAb Investigated by Mobility-Selective CIU and Tandem-TIMS**; Fanny C Liu[1]; Jusung Lee[1]; Thais Pedrete[1]; Christian Bleiholder[1]; *[1]Florida State University - Department of Chemistry and Biochemistry, Tallahassee, FL*

TP 658 **A middle-level approach to simplify sample preparation and data analysis for characterization of the fusion protein blinatumomab**; Lucy Fernandes[1]; Andreas Nägeli[2]; Magdalena Widgren-Sandberg[2]; Antony Harvey[1]; *[1]ProteinMetrics LLC, Cupertino, CA; [2]Genovis, Kävlinge, Sweden*

TP 659 **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*

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TP 660 **Probing structural dynamic changes of dimeric nitric oxide synthase protein in response to external cues by quantitative cross-linking mass spectrometry**; Ting Jiang[1]; Guanghua Wan[1]; Haikun Zhang[1]; Eric Underbakke[2]; Changjian Feng[1]; *[1]UNM College of Pharmacy, Albuquerque, NM; [2]Iowa State University, Ames, IA*

TP 661 **Studying the conformational interplay of different amyloid β peptides with native ion mobility – mass spectrometry**; Tanja Habeck[1]; Silvana Smilla Zurmühl[1]; Edvaldo Vasconcelos Soares Maciel[1]; Frederik Lermyte[1]; *[1]Technical University of Darmstadt, Clemens-Schöpf-Institute for Organic Chemistry and Biochemistry, Darmstadt, Germany*

TP 662 **The functional proteome landscape in aging**; Xiaojing Sui; *Northwestern University, Evanston, IL*

TP 663 **Probing the formation of heterogenous photosynthetic antenna complexes from blue-green algae using native mass spectrometry**; Jaspreet K Sound[1]; Giorgio Bianchini[2]; Thrupthi Ashok[1]; Patricia Sánchez-Baracaldo[2]; Aneika C Leney[1]; *[1]School of Biosciences, University of Birmingham, Birmingham, United Kingdom; [2]School of Geographical Sciences, University of Bristol, Bristol, United Kingdom*

TP 664 **Comprehensive analysis of SARS-CoV-2 Spike structure and function following genetic reversion reveals contribution of D614G mutation**; Lindsay E Nyhoff[1]; Christopher A. Haynes[1]; Jakub Baudys[1]; Theodore R. Keppel[1]; Sarah H. Osman[1]; John R. Barr[1]; Dongxia Wang[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

TP 665 **Expanding native mass spectrometry capabilities for soluble and membrane proteins using a quadrupole-ion mobility-time-of-flight mass spectrometry system**; Brad Williams[1]; Dale A Cooper-Shepherd[2]; Mario Hensen[3]; Jonathan T. S. Hopper[3]; James I. Langridge[4]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom; [3]OMass Therapeutics, Oxford, United Kingdom; [4]Waters Corporation, Wilmslow, United Kingdom*

TP 666 **Using In Vivo Intact Structure for System-wide Quantitative Analysis of Changes in Proteins**; Ahrum Son[1]; Hyunsoo Kim[1, 2]; Jolene K. Diedrich[1]; Casimir Bamberger[1]; Daniel B. Mcclatchy[1]; John R. Yates III[1]; *[1]Scripps Research, San Diego, California; [2]Chungnam National Univeristy, Daejeon, South Korea*

TP 667 **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[1, 2]; Paulo E. Santo[3, 4]; Marie-Eve Chagot[5]; Bruno Charpentier[5]; Tiago M. Bandeiras[3, 4]; Xavier Manival[5]; Oscar Hernandez-Alba[1, 2]; Sarah Cianférani[1, 2]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, IPHC UMR 7178, Université de Strasbourg, CNRS, Strasbourg, France; [2]Infrastructure Nationale de Protéomique ProFI – FR2048, Strasbourg, France; [3]iBET, Instituto de Biologia Experimental e Tecnológica, Oeiras, Portugal; [4]Instituto de Tecnologia Química e Biológica António Xavier, Universidade Nova de Lisboa, Oeiras, Portugal; [5]IMoPA, CNRS, Université de Lorraine, Nancy, France*

TP 668 **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 669 **Digital Quadrupole Isolation with Electron Capture Dissociation Provides Structure Information on the Transthyretin Tetramer**; Carter Lantz[1]; Robert Schrader[1]; Joseph Meeuwsen[2]; Rachel Franklin[2]; Noah Goldberg[2]; David Russell[1]; *[1]Texas A&M University, College Station, TX; [2]Agilent Technologies, Santa Clara, CA*

TP 670 **Probing Relative Flexibility of Apolipoprotein E Surface Regions by Non-specific Limited Proteolysis coupled with Mass Spectrometry**; Zachary P Del Mundo[1]; Vu Ngoc Huong Tran[1]; Haiyan Lu[1]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison School of Pharmacy, Madison, WI; [2]University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin*

TP 671 **Combining structural modeling and cross-linking mass spectrometry reveals protein binding sites within disordered regions**; Julia Ruta[1]; Cong Wang[1]; Ying Zhu[1];

Pin-Lian Jiang[1]; Boris Bogdanow[1]; Fan Liu[1, 2]; *[1]Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; [2]Charité, Universitätsmedizin Berlin, Berlin, Germany*

TP 672 **Structural Proteomics Derived Structural-Activity Relationships of Novel PPARg Inverse Agonists**; Kuang-Ting Kuo[1, 2]; Bilel Bdiri[3]; Yuanjun He[3]; Marcel Koenig[3]; Theodore Kamenecka[3]; Patrick R. Griffin[1, 2, 3]; *[1]Department of Molecular Medicine, The Scripps Research Institute, Jupiter, FL; [2]Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; [3]Department of Molecular Medicine, The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL*

TP 673 **Effect of Ligands on Transthyretin Structure & Sub-Unit Exchange Mechanism Monitored by Native Ion Mobility Mass Spectrometry**; Robert Rider[1]; Carter Lantz[1]; Sangho Yun[1]; David H Russell[1]; *[1]Texas A&M University, College Station, TX*

TP 674 **Deep Ultraviolet Laser Protein Footprinting**; Kermit K. Murray[1]; Oluwatosin A. Ogundairo[1]; Kadeem Hayes[1]; *[1]Louisiana State University, Baton Rouge, LA*

TP 675 **RAMP it up! Exploring conformational dynamics of the amylin 3 receptor (AMY3R) using HDX-MS**; Cameron J Fairweather[1, 2]; Xin Zhang[1, 2]; Daniel J Garama[3]; Patrick M Sexton[1, 2]; Denise Wootten[1, 2]; Tracy M Josephs[1, 2]; *[1]Monash University, Parkville, Australia; [2]ARC Centre for Cryo-electron Microscopy of Membrane Proteins, Parkville, Australia; [3]Hudson Institute of Medical Research, Clayton, Australia*

TP 676 **Utilizing U-Shaped Mobility Analyzer (UMA) for High Performance Dust-Mite AllergenDer p2 Quality Control**; Zixin Liang[1]; Kang Guo[2]; Xiaoqiang Zhang[2]; Wenjian Sun[2]; Huilin Li[1]; *[1]Sun Yat-Sen University, Guangzhou, China; [2]Shimadzu Research laboratory (Shanghai) Co. Ltd., Shanghai, China*

TP 677 **Covalent Modification of Cytochrome c During Thermal Unfolding and their Implications for Thermodynamic Stability Measurements**; Evelyn H MacKay-Barr[1]; Lars Konermann[1]; *[1]University of Western Ontario, London, Ontario*

TP 678 **Mass spectrometry-based footprinting methods reveals the effect of redox partner binding on the conformational dynamics of cytochrome P450**; Mengqi Chai[1]; Sarah Burris-Hiday[2]; Emily E. Scott[2]; Michael L. Gross[1]; *[1]Washington University in St. Louis, Saint Louis, MO; [2]University of Michigan, Ann Arbor, MI*

TP 679 **Transient multimers modulate conformer abundances of prion protein monomer through conformational selection: an ion mobility and mass spectrometry study**; Guillaume Van Der Rest[1]; Human Rezaei[2]; Frederic Halgand[3]; *[1]Institut de Chimie Physique, Orsay, France; [2]INRAE, Jouy en Josas, France; [3]CNRS / Universite Paris Saclay, Orsay, France*

TP 680 **Structural characterization of the C1 and C2 epitopes of coagulation factor VIII by X-ray Footprinting and Mass Spectrometry**; Sathi Paul[1]; Kenneth Childers[2]; Darren Kahan[3]; Susan Marqusee[3]; P. Clint Spiegel Jr[2]; Corie Y Ralston[1]; Sayan Gupta[1]; *[1]Lawrence Berkeley National Laboratory, Berkeley, CA; [2]Western Washington University, Bellingham, WA; [3]University of California, Berkeley, Berkeley, CA*

TP 681 **Development of a Web-Based Visualization tool for robust interpretation of Protein Cross-Linking**; Sanjeeva Srivastava[1]; Deeptarup Biswas[1]; Sanjyot Vinayak Shenoy[1]; Kamal Mandal[2]; Arthur Zalevsky[3]; Ishan Upadhyay[1]; Ayushi Verma[1]; Audrey Kishishita[4]; Andrej Sali[4]; Arun Wiita[4]; *[1]IIT Bombay, Mumbai, India; [2]Gujarat Biotechnology University, Ahmedabad, India; [3]University of California San Francisco, San Francisco, CA; [4]University of California-San Francisco, San Francisco, CA*

TP 682 **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[1]; Line G Kristensen[1]; Sathi Paul[1]; Brandon Russell[1]; Corie Y Ralston[1]; *[1]Lawrence Berkeley National Laboratory, Berkeley, CA*

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TP 683 **Above-Filter Digestion Proteomics (AFDIP) identifies drug targets and estimates ligand binding site**; Bohdana Sokolova[1]; Amir Ata Saei[1]; Hassan Gharibi[1]; Maryam Jafari[1]; Hezheng Lyu[1]; Massimiliano Gaetani[1]; Roman Zubarev[1]; *[1]Karolinska Institutet, Stockholm, Sweden*

TP 684 **Protein a-N-methylation promotes nucleocytoplasmic transport of aminoacyl-tRNA**; Quanqing Zhang[1]; Yinsheng Wang[1]; *[1]UC Riverside, Riversdie, CA*

TP 685 **Automated High-throughput Activity-based Protein Profiling Facilitates Covalent Drug Discovery**; Yumeng Li[1]; Zhenze Jiang[1]; *[1]Roche, Shanghai, China*

TP 686 **Enabling activity-based protein profiling (ABPP) for drugs that form disulfides: identification of off-targets for ALS and alcohol abuse drugs**; Durgalakshmi Sivasankar[1]; Wensheng Yang[1]; Jeffrey Agar[1]; *[1]Northeastern University, Boston, MA*

TP 687 **High-throughput profiling of compound-induced proteome thermal stability changes**; Alexey Chernobrovkin[1]; Daniel Martinez Molina[1]; *[1]Pelago Bioscience AB, Solna, Sweden*

TP 688 **Getting the Most Out of Thermal Proteome Profiling: Comparison of R Packages for Data Analysis**; Connor P Jewell[1]; Massimiliano Bissa[2]; Andrew J Perciaccante[1]; Genoveffa Franchini[2]; Daniel H Appella[3]; Lisa M Jenkins[1]; *[1]Laboratory of Cell Biology, Center for Cancer Research, National Cancer Institute, Bethesda, MD; [2]Vaccine Branch, Center for Cancer Research, National Cancer Institute, Bethesda, MD; [3]Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD*

TP 689 **Chemical Proteomic Strategy Utilizing a Photoreactive Chloroalkane Capture Tag for Target Discovery**; Alba Katiria González Rivera[1]; Robin Hurst[1]; Sergiy Levin[2]; Michael M. Rosenblatt[1]; Rachel Friedman Ohana[1]; *[1]Promega Corporation, Madison, WI; [2]Firmenich SA, R&D North America, San Diego, California*

TP 690 **Unbiased identification of SAMT-247 reaction sites on proteins in cell lysates**; Tapan K. Maity[1]; Connor P. Jewell[1]; Andrew J. Perciaccante[1]; Daniel H. Appella[2]; Lisa M. Jenkins[1]; *[1]Laboratory of Cell Biology, Center for Cancer Research, National Cancer Institute, Bethesda, MD; [2]National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD*

TP 691 **Rescue of ΔF508-CFTR trafficking in cystic fibrosis through a QPCT-dependent pathway**; Le Sun; *the Scripps Research Institute, San Diego, CA*

TP 692 **Misfolded Protein Profiling Reveals the Protein Targets of Cellular Manganese and Vanadium Exposure**; Guy M. Quanrud[1]; Macon Abernathy[1]; Samantha C. Ying[1]; Joseph Genereux[1]; *[1]University of California, Riverside, Riverside, CA*

TP 693 **Confluence of Safeguards: A Chemoproteomic Platform for Highly Sensitive and Selective Citrulline Mapping in Alzheimer's Disease**; Wei Wilson Li[1]; Zexin Zhu[1]; Haiyan Lu[1]; Zicong Wang[1]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison School of Pharmacy, Madison, WI; [2]University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin*

TP 694 **Uniting global and subcellular-localized redox proteomics to uncover redox-sensitive cysteine regulators of stress granule dynamics**; Ashley Julio[1]; Katarina Cohen[1]; Keriann M Backus[1]; *[1]UCLA, Los Angeles*

TP 695 **Cysteine-reactive electrophilic compounds remodel the proteome by modulating cellular proteostasis processes**; Flowreen Shikwana[1]; Ashley Julio[1]; Cindy Truong[1]; Nikolas Burton[1]; Emil R. Dominguez[1]; Alexandra C.

Turmon[1]; Jian Cao[1]; Keriann M Backus[1]; *[1]University of California, Los Angeles, Los Angeles, CA*

TP 696 **CIAA: Integrated Proteomics and Structural Modeling for Predicting Cysteine Reactivity with Iodoacetamide Alkyne**; Lisa M Boatner[1]; Jerome Eberhardt[2]; Jose O Castellon[1]; Flowreen Shikwana[1]; Kendall N Houk[1]; Stefano Forli[2]; Keriann M Backus[1]; *[1]University of California Los Angeles, Los Angeles, CA; [2]Scripps Research Institute, San Diego*

TP 697 **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 698 **Mass Spectrometry-Aided Identification and Characterization of Helicase Binders That Can Irreversibly Bind to a Transient Pocket and Inhibit Activity**; Jeremiah J Bowers[1]; Doug McLaughlin[2]; Dave M. Garby[1]; Brian Sosa[2]; William LaMarr[1]; Peter Rye[1]; Bini Ramachandran[1]; *[1]Momentum Biotechnologies, Billerica, MA; [2]MOMA Therapeutics, Cambridge, MA*

TP 699 **Application of chemoproteomics for the preclinical characterization of highly selective and potent covalent BTK inhibitors**; Bekim Bajrami; *Biogen, Cambridge, MA*

TP 700 **Unbiased compound selectivity profiling using high throughput CETSA MS**; Alexey Chernobrovkin[1]; Tuomas A Tolvanen[1]; Tomas Friman[1]; Christina Velasco[1]; Daniel Martinez Molina[1]; *[1]Pelago Bioscience AB, Solna, Sweden*

TP 701 **An Automated Proteome Integral Solubility Alteration (PISA) Workflow Using DIA for Increased Throughput and Robustness**; Keith D Rivera[1]; Isabelle A Kressy[1]; Natalie M Clark[1]; D. R. Mani[1]; Namrata D. Udeshi[1]; Steven A Carr[1]; *[1]Broad Institute, Cambridge, MA*

TP 702 **Bromo-desthiobiotin tag (Br-DTB) for unbiased profiling of chemical modification sites in human proteome**; Bibhuti Bhusana Palai[1]; Zongtao Lin[1]; Benjamin A. Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

TP 703 **Comparing serum protein profiles of Homo sapiens with Pan troglodytes via Label-free MS proteomics: How similar are we?**; Marcos N Eberlin[1]; Mariana Sá[2]; Iasmim Lopes Lima[1]; Thais Regiane Cataldi[3]; Esther Olabisi-Adeniyi[2]; Jennifer Geddes-McAlister[2]; *[1]Mackenzie University, São Paulo, Brazil; [2]University of Guelph, GUELPH, ON; [3]Universidade de São Paulo, Piracicaba, Brazil*

TP 704 **Proteomics and bioinformatics reveal anandamide antinociceptive effects are mediated by vanilloid receptors in Caenorhabditis elegans**; Marzieh Abdollahi[1]; Jennifer Ben Salem[1]; Jesus D Castano[1]; Francis Beaudry[1]; *[1]Universite de Montreal, St-Hyacinthe, QC*

TP 705 **Exploring sample preparation workflows and instrument acquisitions for chemoproteomic global protein profiling**; Taylur P. Ma[1]; Meena Choi[1]; Felipe Da Veiga Leprevost[1]; Nicolas Hartel[2]; Jana Richter[2]; Hanna G. Budayeva[1]; *[1]Genentech, Inc., South San Francisco, CA; [2]ThermoFisher Scientific, San Jose, CA*

TP 706 **Polymerase κ Recruits DDX23 to Promote R-loop Resolution**; Feng Tang[1]; Yinan Wang[2]; Yinsheng Wang[2]; *[1]University of California, riverside, Riverside, CA; [2]UC Riverside, Riversdie, CA*

TP 707 **An ultra-deep, cysteine-profiling approach for chemoproteomics powered by TMT and the new Astral mass analyzer**; Ka Yang[1]; Qing Yu[1]; Shane L. Dawso[1]; Rebecca L. Whitehous[1]; Lu Zhang[2]; Jeffrey G. Martin[2]; Douglas S. Johnson[2]; Joao A. Paulo[1]; Steven Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Biogen, Cambridge, MA*

TP 708 **Leveraging Data Independent Acquisition (DIA) for Cysteine Targeting and Proteome Profiling**; Lara Holoidovsky[1]; Tianyang Yan[1]; Weixian Deng[1]; James Wohlschlegel[1]; Keriann M Backus[1]; *[1]UCLA, Los Angeles*

TP 709 **Fast Photochemical Iodination and Capture by Suzuki as a Novel Tyrosine Chemoproteomics Method**; Miranda Villanueva[1]; Nikolas Burton[1]; Andrew Becker[1]; Eli Biletch[1]; Sho Takechi[1]; Keriann M Backus[1]; *[1]UCLA, Los Angeles, CA*

TP 710 **Generating Cysteine-Trypsin Cleavage Sites With 2-Chloroacetamidine Capping**; Samuel Ofori[1]; Heta Desai[2]; Flowreen Shikwana[1]; Lisa Boatner[1]; Jose O Castellon[1]; Keriann M Backus[1]; *[1]UCLA, Los Angeles, California; [2]Gristone Bio, Boston, USA, Massachusetts*

TP 711 **Probing the Target Site for a Promising Acaricide to Tackle Varroa Mites in Honeybee Colonies**; Osei Boakye Fordwour[1]; Niloufar Choubdar[2]; Laura Gleeson[2]; Erika Plettner[2]; Leonard J Foster[1]; *[1]UBC, Vancouver, BC; [2]Simon Fraser University, Burnaby, BC*

TP 712 **From seeding to separation: a 96-well format sample preparation protocol for cell-based high throughput proteomics**; Julia E Robbins[1]; Andrea I Gutierrez[2]; J. Sebastian Paez[2]; Daniele Canzani[2]; Bodhi Hueffmeier[2]; Brian McEllin[2]; Carolyn Allen[2]; Yang Gao[2]; Tonibelle Gatbonton-Schwager[2]; William E Fondrie[2]; Alexander J Federation[2]; Lindsay K Pino[2]; *[1]Talus Bioscience, Seattle; [2]Talus Bioscience, Seattle, WA*

TP 713 **A Chemoproteomic Approach to Identifying Biologically Active Cyclic Peptides**; Katrina H. Andrews[1]; Haley Gauer[1]; Nikolas R. Burton[1]; Keriann M. Backus[1]; *[1]University of California, Los Angeles, Los Angeles, CA*

TP 714 **Developing a minimalist proximity labeling method using the short tetracysteine tag**; Elijah B. Biletch[1, 2]; Andrew P. Becker[1, 2]; Tomoyuki Fukuta[3, 4]; Keriann M. Backus[1, 2]; *[1]Department of Biological Chemistry, David Geffen School of Medicine, UCLA, Los Angeles, CA; [2]Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA; [3]Department of Chemistry, School of Science, The University of Tokyo, Tokyo, Japan; [4]Graduate School of Pharmaceutical Sciences, The University of Tokyo, Tokyo, Japan*

TP 715 **Advancing the discovery of novel senolytics through cysteine-focused activity-based protein profiling**; Matthew White[1, 2]; Jesús Gil[2, 3]; Edward W. Tate[4, 5]; *[1]Imperial College London, London, United Kingdom; [2]MRC London Institute of Medical Sciences (LMS), London, United Kingdom; [3]Institute of Clinical Sciences (ICS), Faculty of Medicine, Imperial College London, London, United Kingdom; [4]Imperial College London, London, United Kingdom; [5]Francis crick institute, London, United Kingdom*

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TP 716 **Proteomic evidence that Heimdall, an alternative protein from a non-coding RNA knockout, switches astrocytes to a neural stem cell phenotype**; Alice Capuz[1, 2]; Isabelle Fournier[1]; Franck Rodet[1]; Michel Salzet[1]; *[1]Laboratoire PRISM, Inserm U1192, Université de Lille, Villeneuve d'Ascq Cedex, France; [2]Brigham and Women's Hospital, Boston, MA*

TP 717 **Data-independent acquisition mass spectrometry analysis of serum proteomic profiles in chronic obstructive pulmonary disease**; Wen-Yi Liu[1]; Sheng-Ming Wu[1]; Kuan-Yuan Chen[1]; Kang-Yun Lee[1]; Chia-Li Han[1]; *[1]Taipei Medical University, Taipei, Taiwan*

TP 718 **Ultra-deep Monitoring of Human and Pig Proteins in Blood Serum Yields Novel Insights into the Dynamics of Pig Kidney Xenotransplantation**; Alexey Stukalov[1]; Brittany Lee[1]; Khatereh Motamedchaboki[2]; Brian D. Piening[3]; Eloi Schmauch[4]; Simon Williams[5, 6]; Ian Jaffe[3, 5]; Maedeh Mohebnasab[7]; Alexa Dowdell[3]; Adam Griesemer[5, 6]; Karen Khalil[5, 6]; Jacqueline I. Kim[3, 5]; David Ayares[8]; Marc Lorber[9]; Massimo Mangiola[5, 10]; Vasishta Tatapudi[5, 11]; Jeffrey M. Stern[5, 6]; Jef D. Boeke[12]; Harvey I. Pass[6]; Robert A. Montgomery[5, 6]; Serafim Batzoglou[1]; Asim Siddiqui[1]; Brendan J. Keating[5, 6]; *[1]Seer Inc., Redwood City, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Earle A. Chiles Research Institute, Providence Cancer Institute, Portland, OR; [4]Broad Insitute of MIT and Harvard, Boston, MA; [5]NYU Langone Transplant Institute, NYU Langone Health, New York, NY; [6]Department of Surgery, NYU Grossman School* *of Medicine, New York, NY; [7]Division of Molecular & Genomic Pathology, University of Pittsburgh Medical Center, Pittsburgh, PA; [8]Revivicor Inc., Blacksburg, VA; [9]United Therapeutics, Silver Spring, MD; [10]Department of Pathology, NYU Grossman School of Medicine, New York, NY; [11]Department of Medicine, NYU Grossman School of Medicine, New York, NY; [12]Institute for Systems Genetics, NYU Langone Health, New York, NY*

TP 719 **Large-scale pan-cancer study elucidates the proteomic profile of 1261 FFPE tumour samples**; Stephan Eckert[1, 2]; Johanna Tueshaus[1]; Marius Schliemann[1]; Matthew The[1]; Peer-Hendrik Kuhn[3]; Carolin Mogler[3]; Bernhard Kuster[1, 2, 4]; *[1]Technical University of Munich (TUM), Freising, Germany; [2]DKFZ German Cancer Research Center, Heidelberg, Germany; [3]Technical University of Munich (TUM), Munich, Germany; [4]Bavarian Center for Biomolecular Mass Spectrometry (BayBioMS), Freising, Germany*

TP 720 **Differentiating AL amyloidosis from immunoglobulin light chain deposition disease utilizing histopathology and mass spectrometry-based proteomics**; A Cooper Walland[1]; Anna Liu[1]; Mirian Barbosa[1]; Ahmet Dogan[1]; Jessica Chapman[1]; *[1]Memorial Sloan Kettering Cancer Center, New York, NY*

TP 721 **Biomarker Discovery and Quantitation Guided by a Data Independent Acquisition (DIA) Mass Spectrometry Technique**; Ling Li[1]; Sumit Bhutada[2]; Nicolas Piuzzi[3]; Belinda Willard[1]; Suneel Apte[2]; *[1]Department of Shared Laboratory Resources, Cleveland Clinic, Cleveland, Ohio; [2]Department of Biomedical Engineering, Cleveland Clinic, Cleveland, Ohio; [3]Department of Orthopaedic Surgery, Cleveland, Ohio*

TP 722 **Standardized, fully automated undepleted plasma and MagNet enrichment workflows enabled by the Evotip Pure**; Joel Vej-Nielsen[1]; Magnus Huusfeldt[1]; Stoyan Stoychev[1]; Dorte B. Bekker-Jensen[1]; Nicolai Bache[1]; *[1]Evosep, Odense, Denmark*

TP 723 **IonStar-based Clinical Proteomics Pipeline Enables Identification of Novel Biomarkers for Bacterial Exacerbation of Chronic Obstructive Pulmonary Disease**; Xiaoyu Zhu[1]; Shuo Qian[2]; Shichen Shen[1]; Sanjay Sethi[1]; Gordon Broderick[3]; Jun Qu[1, 4]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell Park Comprehensive Cancer Center, Buffalo, NY; [3]Rochester General Hospital, Rochester, New York; [4]New York State Center of Excellence in Bioinformatics and Life Sciences, buffalo, New York*

TP 724 **Optimizing LC-MS/MS settings for plasma proteomics analysis with cap-flow LC separation and dia-PASEF**; Andreas Schmidt[1]; Claudia Martelli[2]; Raphael Schuster[1]; Schmit Pierre-Olivier[3]; Markus Lubeck[1]; *[1]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; [2]Bruker Switzerland AG, Faellanden, Switzerland; [3]Bruker Daltonique S.A., Wissembourg, France*

TP 725 **Quantification of Her2 expression in Her2-low tumors by targeted mass spectrometry**; Negarsadat Mostolizadeh[1]; Neginsadat Mostolizadeh[1]; Gerald Batist[2, 3, 4]; Mark Basik[2, 3, 4, 5]; Christoph H. Borchers[1, 2, 3, 6]; *[1]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [2]Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; [3]Division of Experimental Medicine, McGill University, Montreal, QC; [4]Department of Oncology, McGill University, Montreal, QC; [5]Department of Surgery, McGill University, Montreal, QC; [6]Department of Pathology, McGill University, Montreal, QC*

TP 726 **No automation? No problem! An optimized, simplified workflow for the targeted proteomic analysis of fibrinogen in 4,200 plasma samples**; Carly A. I. Twigg[1]; Joohyun Ryu[1]; Stefani N. Thomas[1]; *[1]Department of Laboratory Medicine and Pathology, University of Minnesota School of Medicine, Minneapolis, MN*

TP 727 **Novel scavengers unbiasedly quadruple FFPE protein yields for clinical proteogenomics**; Matthew Holt[1]; Craig T. Vollert[1]; George Miles[1, 2]; Eric C. Chang[1, 3]; Charles E Foulds[1, 4]; Bing Zhang[1, 2]; *[1]Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; [2]Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, Texas; [3]Department of Molecular and Cellular Biology, Baylor College of Medicine, Houston, Texas; [4]Department of Medicine, Baylor College of Medicine, Houston, Texas*

TP 728 **Optimizing Capivasertib Response Prediction in Cancer: Unveiling Resistance Mechanisms through Precision Proteomics**; Neginsadat Mostolizadeh[1]; Negarsadat Mostolizadeh[1]; Gerald Batist[2, 3, 4]; Mark Basik[3, 4, 5, 6]; Christoph H. Borchers[1, 2, 3, 7]; *[1]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [2]Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; [3]Division of Experimental Medicine, McGill University, Montreal, QC; [4]Department of Oncology, McGill University, Montreal, QC; [5]Gerald Bronfman Department of Oncology, McGill University, Montreal, QC; [6]Department of Surgery, McGill University, Montreal, QC; [7]Department of Pathology, McGill University, Montreal, QC*

TP 729 **Identification of 15-keto-PGE2 post-translational protein modifications by LC/MS/MS to study an anti-inflammatory therapy**; Fu-An Li[1]; Ling-Hui Wang[1]; *[1]Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan*

TP 730 **Efficient analysis of phosphopeptides from lung cancer tissues on a silica-based monolithic column and timsTOF**; Bella Bruszel[1]; Fanni Bugyi[2]; Goran Mitulovic[3]; Michael Krawitzky[3]; Gary Kruppa[4]; Armel Nicolas[1]; Lilla Turiak[2]; *[1]Institute of Science and Technology, Maria Gugging, Austria; [2]HUN-REN Research Centre for Natural Sciences, Budapest, Hungary; [3]Bruker Switzerland AG, Faellanden, Switzerland; [4]Bruker S.R.O., Brno, Czech Republic*

TP 731 **Turbocharging Discovery: Crafting a High-Speed, High-Efficiency Monolithic Column for Breakneck Single-Cell Analysis**; Ruben Shrestha[1]; Michael Krawitzky[2, 3]; Simion Kreimer[4]; Goran Mitulovic[3]; Ali Haghani[4]; Jennifer E. Van Eyk[4]; Gary Kruppa[5]; *[1]Bruker Scientific LLC, San Jose, CA; [2]Bruker Daltonics, San Jose, CA; [3]Bruker Switzerland AG, Faellanden, Switzerland; [4]Cedars-Sinai Medical Center, Los Angeles; [5]Bruker S.R.O., Brno, Czech Republic*

TP 732 **Development and application of quantitative proteomics for assessing preclinical and clinical pharmacodynamic activity of a potent STAT3 protein degrader**; Eric Kuhn[1]; Sarah Martinez[1]; Joyoti Dey[1]; Alyssa Fasciano[1]; Christine Klaus[1]; Susanne Breitkopf[1]; Yatao Shi[1]; Dirk Walther[1]; Yi-Ting Wang[1]; Chris Browne[1]; Dapeng Chen[1]; Beccy Mosher[1]; Jared Gollob[1]; Juliet Williams[1]; Kirti Sharma[1]; *[1]Kymera Therapeutics, Watertown, MA*

TP 733 **A multimodal approach determining effects of estrogen receptor alpha (ERα) inhibition in mouse models of benign prostatic hyperplasia**; Hannah Miles[1, 2, 3]; Elliot Patrenets[3, 4]; William A. Ricke[1, 2, 3, 5]; Lingjun Li[6, 7]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of Urology, UW-Madison, Madison, WI; [3]George M. O'Brien Urology Research Center, UW-Madison, Madison, WI; [4]Department of Integrative Biology, UW-Madison, Madison, WI; [5]School of Medicine and Public Health, UW-Madison, Madison, WI; [6]School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin; [7]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

TP 734 **Advancement in nanoparticle-based proteomic analysis of whole blood obtained from various dried blood spot collection devices**; Maedeh Zamani[1]; Brittany Lee[1]; Shao-Yung Chen[1]; Shadi Ferdosi[1]; Xiaoyuan Zhou[1]; Daniel Hornburg[1]; Aaron Steven Gajadhar[1]; *[1]Seer Inc., Redwood City, CA*

TP 735 **LC-SRM and machine learning allowing fast detection of urinary tract infections**; Clarisse Gotti[1]; Florence Roux-Dalvai[1]; Antoine Lacombe-Rastoll[1]; Cristina Jacob[2]; Eve Bérubé[3]; Maurice Boissinot[3]; Michel G. Bergeron[3]; Neloni Wijeratne[2]; Claudia Martins[2]; Arnaud Droit[1]; *[1]Proteomics Platform and Computational Biology laboratory, CHU de*

Québec Université Laval Research Center, Québec, QC; [2]Thermo Fisher Scientific, San Jose, CA; [3]Infectiology Research Centre, CHU de Québec Université Laval Research Center, Québec, QC

TP 736 **In-depth proteomic analysis of mouse inner ear for the studies of age-related hearing loss**; Samon Nagatani[1]; Maiko Okamura[1]; Yoko Fukunaga[2]; Shuji Yamashita[1]; Takashi Nirasawa[3]; Hiroki Kato[4]; Kengo Yoshii[4]; Norio Yamamoto[2, 5]; Masaya Ikegawa[1]; *[1]Doshisha University, Kyotanabe, Japan; [2]Kyoto university, Sakyo-ku, Japan; [3]Bruker Japan K.K., Yokohama, Japan; [4]Kyoto Prefectural University of Medicine, Kamigyo-ku, Japan; [5]Kobe City Medical Center General Hospital, Kobe, Japan*

TP 737 **Utility of novel capillary-based blood collection devices as alternatives to venipuncture for a new MRM clinical proteomic assay**; Sarah Phillips[1]; Abby Richard[1]; Alicia Patrick[1]; Cara Kifer[1]; Danielle Dvorak[1]; Merrie Ann O'Brien[1]; Sierra Whitted[1]; Gary Pestano[2]; Laura Peek[1]; *[1]Biodesix, De Soto, KS; [2]Biodesix, Louisville, CO*

TP 738 **Utility of a Novel Blood Storage Device for Clinical Proteomics and its Effect on the Plasma Proteome**; Colin T McDowell[1]; Amanda Weaver[1]; Gary Pestano[1]; *[1]Biodesix, Louisville, CO*

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TP 739 **Multi-omics reveals that Sirt2 and Sirt5 differentially control macrophage polarization**; Hui Tang[1]; Tuvshintugs Baljinnyam[1]; Abhishek Mishra[2]; Chinnaswamy Jagannath[2]; Kangling Zhang[1]; *[1]University of Texas Medical Branch at Galveston, Galveston, TX; [2]Houston Methodist Research Institute & Weill Cornell Medical College, Houston, Texas*

TP 740 **Kinetic analysis and ultrasensitive detection of SARS-CoV-2 3CLpro-mediated proteolysis.**; Peter A Bell[1]; Kevin Yang[2]; Reinhild Kappelhoff[1]; Julia Kraegenbring[3]; Amirmansoor Hakimi[2]; Hugo Cesar Ramos De Jesus[1]; Brett Larsen[4]; Rosa Viner[2]; Christopher M Overall[1]; *[1]University of British Columbia, Vancouver, BC; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific GmbH, Bremen, Germany; [4]Thermo Fisher Scientific, Toronto, ON*

TP 741 **Polymycovirus Alteration of Virulence Factors in Aspergillus fumigatus: A Mass Spectrometric Proteomics Study** ; Catalina Avendaño[1]; Sydney Nguyen[1]; Ioly Kotta-Loizou[2, 3]; Gabriele Sass[4]; Daniel Röth[1]; David A. Stevens[4, 5]; Markus Kalkum[1]; *[1]City of Hope, Beckman Research Institute. Department of Immunology and Theranostics, Duarte, CA; [2]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; [3]University of Hertfordshire, School of Life and Medical Sciences, Department of Clinical, Pharmaceutical and Biological Science, London, United Kingdom; [4]California Institute for Medical Research, San Jose, CA; [5]Stanford University School of Medicine, Division of Infectious Diseases and Geographic Medicine, Stanford, CA*

TP 742 **Targeting G9a Regulated m6A RNA Modification Pathway to Hinder SARS-CoV-2 Replication**; Adil Muneer[1]; Ling Xie[2]; Feng Zhang[3]; Xuping Xie[4]; John A Wrobel[2]; Yan Xiong[5]; Xufen Yu[5]; Charles Wang[6]; Ciprian Gheorghe[6]; Ping Wu[4]; Hongjun Song[3]; Jin Jian[5]; Pei-Yong Shi[4]; Xian Chen[2]; *[1]University of North Carolina Chapel Hill, Chapel Hill, NC; [2]University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]University of Pennsylvania, Philadelphia, PA; [4]University of Texas Medical Branch at Galveston, Galveston, TX; [5]Icahn School of Medicine at Mount Sinai, New York, NY; [6]Loma Linda University, Loma Linda, CA*

TP 743 **Vitamin B12 physiology and metalloproteome changes in the pathogen Pseudomonas aeruginosa across environmental gradients**; Viktoria Steck[1]; Matthew R. McIlvin[1]; Mak A Saito[1]; *[1]Woods Hole Oceanographic Institution, Falmouth, MA*

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TP 744 **A new strategy for screening disease-associated proteins by MS based on drug and protein interactions**; Weibing Zhang[1]; Yini Pan[1]; Zhenxin Wang[2]; Zhichao Yan[1]; Haofan Sun[3]; Lingyi Zhang[1]; *[1]East China University of Science and Technology, Shanghai, China; [2]Zhongshan Hospital Fudan University, Shanghai, China; [3]Beijing Proteome Research Center, Beijing, China*

TP 745 **Real-time Isotopic Signature Targeted Profiling**; Guogeng Jia[1]; Yicheng Liu[1]; Tianyu Feng[1]; Chu Wang[1]; *[1]Peking University, Beijing, China*

TP 746 **Pursuing Options In Parallel: Multiplexed In Vivo Screening Using Peptide Tagging with mRNA**; Jason Thall[1]; Lisa Crawford[1]; Jonathan Hoggatt[1]; *[1]Moderna, Cambridge, MA*

TP 747 **Bottom-Up Proteomics of Human Keratinocytes Exposed to 4,4'-Methylene Diphenyl Diisocyanate-Glutathione Conjugates by Off-Line MuDPIT**; Brandon F Law[1]; Chen-Chung Lin[1]; Justin M. Hettick[1]; *[1]Centers for Disease Control, NIOSH, Morgantown, WV*

TP 748 **Improving complex phosphopeptide characterization with hybrid electron activated dissociation and collision-induced dissociation fragmentation**; Patrick Pribil[1]; Loren Olsen[2]; Jeremy Potriquet[3]; Daniel Winter[4]; *[1]SCIEX, Concord, ON; [2]SCIEX, Redwood City, CA; [3]SCIEX, Mulgrave, Australia; [4]All G Foods, Waterloo, Australia*

TP 749 **An Automated Sample Preparation Workflow for Proteomic Profiling of Membrane-Bound Vesicles from Urine**; Ireshyn Govender[1]; Sindisiwe Buthelezi[2]; Previn Naicker[2]; Andrea Ellero[1, 3]; Justin Jordaan[1]; Stoyan Stoychev[1, 4]; *[1]ReSyn Biosciences, Pretoria, South Africa; [2]Council for Scientific and Industrial research, Pretoria, South Africa; [3]University of Pretoria, Pretoria, South Africa; [4]Evosep, Odense, Denmark*

TP 750 **Refining data acquisition parameters for low concentration proteomics using a Vanquish™ Neo LC coupled to an Orbitrap Eclipse™ Mass Spectrometer**; Theodore R. Keppel[1]; Yu Zhou[1]; Jakub Baudys[1]; Dongxia Wang[1]; John R. Barr[1]; *[1]CDC, Atlanta, GA*

TP 751 **High-throughput Workflow for Deep Analysis of Human Serum Proteome by Mass Spectrometry**; Yanyan Qu[1]; Ravi Tharakan[1]; Yuhong Fang[1]; Claire Weber[2]; Emily Chew[2]; Christopher A LeClair[1]; Dingyin Tao[1]; *[1]National Center for Advancing Translational Sciences, NIH, Rockville, MD; [2]National Eye Institute, NIH, Bethesda, MD*

TP 752 **Development of a Thiol Exchange- and Mass Spectrometry-Based Proteomic Method for the Evaluation of Protein Folding Kinetics**; Yuegi Chen[1]; Terrence G. Oas[1]; Michael C. Fitzgerald[1]; *[1]Duke University, Durham, NC*

TP 753 **High Throughput Abundant Protein Depletion for Plasma Proteomics**; Amarjeet Flora[1]; Anastasia Klenke[1]; Bhavin Patel[1]; Ryan Bomgarden[1]; *[1]Thermo Fisher Scientific, ROCKFORD, IL*

TP 754 **An EasyPep Magnetic solution for automated proteomics sample preparation**; Maowei Dou[1]; Erum Raja[1]; Leigh Foster[1]; Kevin Yang[2]; Amirmansoor Hakimi[2]; Sergei Snovida[1]; Kay Opperman[1]; Bhavin Patel[1]; Ryan Bomgarden[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, San Jose, CA*

TP 755 **Multicolumn Nanoflow Liquid Chromatography System with Accelerated Offline Gradient Generation for Robust and Sensitive Single-Cell Proteome Profiling**; Xiaofeng Xie[1]; Thy Truong[1]; Ryan T. Kelly[1]; Siqi Huang[1]; Madi Johnston[1]; Kei Webber[1]; Lavender Lin[1]; *[1]Brigham Young University, Provo, UT*

TP 756 **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[1]; Elizabeth D. Lightbody[2]; Kirsty Wienand[1]; Hasmik Keshishian[1]; John Thorup[1]; Simone Zhang[1]; Moe Haines[1]; Shankha Satpathy[1]; Francisca Vazquez[1]; Irene M. Ghobrial[2]; Michael A. Gillette[1]; Steven A. Carr[1]; *[1]Broad*

Institute, Cambridge, MA; [2]Dana-Farber Cancer Institute, Boston, MA

TP 757 **Next-generation protein sequencing integrates with top-down and individual ion mass spectrometry to distinguish native and artifactual proteoforms**; Andrew Lee[1]; Kenneth Skinner[2]; Taojunfeng Su[1]; Michael Warchol[2]; Aniel Sanchez[1]; Haidong Huang[2]; Troy D Fisher[1]; Eleonora Forte[1]; Michael A Caldwell[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Quantum-Si Inc., Branford, CT*

TP 758 **Exploring Digestion Enzymes for Online Microdroplet-Enabled Analysis of LC Separated mAbs**; Timothy Yaroshuk[1]; Andrew Schladebeck[1, 2]; Jim Lau[3]; Mike Knierman[3]; Harsha Gunawardena[4]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]Kenvue, Skillman, NJ; [3]Agilent Technologies, Santa Clara, CA; [4]Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania*

TP 759 **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[1]; Khadiza Zaman[2]; Karsten Liegmann[3]; Brian Shofran[3]; Laszlo Prokai[2]; Vladimir Shulaev[1]; *[1]University of North Texas, Denton, TX; [2]University of North Texas Health Science Center, Department of Pharmacology and Neuroscience,, Fort Worth, Texas; [3]Tecan, Baldwin Park, CA*

TP 760 **Advancing Model Organism Plasma/Serum Proteomics with Proteograph XT: A species agnostic platform for deep unbiased proteomics profiling**; Shao-Yung Chen[1]; Wei Jiang[2]; Pierre Mbarushimana[2]; Alexis Jacob[2]; Maedeh Zamani[2]; Ryan Hill[2]; Alexey Stukalov[2]; Xiaoyuan Zhou[2]; Ambika Sundaresan[2]; Dashyanng Kachru[2]; Ryan W. Benz[2]; Aaron Gajadhar[2]; *[1]Seer, Redwood City, CA; [2]Seer, Inc., Redwood City, CA*

TP 761 **Analysis of the workflow involving protein capture using hydrophilic magnetic beads**; Michael Rosenblatt[1]; Chris Hosfield[1]; Zhiyang Zeng[2]; Wenhui Zhou[2]; Marjeta Urh[1]; *[1]Promega Corp, Madison, WI; [2]Promega Corporation, San Luis Obispo, CA*

TP 762 **Characterization of a new ultra-selective, highly active Arginine-C protease for MS-based proteomics**; Tim Heymann[1]; Chris Hosfield[2]; Mike Rosenblatt[2]; Marjeta Urh[2]; Georg Wallmann[1]; Marta Murgia[1]; Matthias Mann[1, 3]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Promega Corporation, Madison, WI 53711; [3]Novo Nordisk Foundation Center for Protein Research (CPR), University of Copenhagen, Copenhagen, Denmark*

TP 763 **Chemical acetylation strategy to access previously unidentified ubiquitination sites in lysine-rich regions of the proteome**; Daryl N. Bulloch[1]; Ishwar Kohale[1]; Han-Yin Yang[1]; Kibeom Kim[1]; Aman Makaju[2]; Matthew J. Rardin[1]; *[1]Amgen, South San Francisco, CA; [2]Amgen, Thousand Oaks, CA*

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764-783

TP 764 **Massively parallel sample preparation for multiplexed single-cell proteomics using nPOP**; Andrew Leduc[1]; Luke Khoury[1]; Joshua Cantlon[2]; Saad Khan[1]; Nikolai Slavov[1, 3]; *[1]Northeastern University, Boston, MA; [2]Scienion US, Tempe, AZ; [3]Parallel Squared Technology Institute, Watertown, MA*

TP 765 **Improving multiplexed single-cell proteomics through the combination of Salud real-time prediction and MSFragger-RTS**; Tommy K. Cheung[1]; Fengchao Yu[2]; Alexey I Nesvizhskii[3]; Christopher Rose[4]; *[1]Genentech, Inc., South San Francisco, CA; [2]University of Michigan, Ann Arbor, MI; [3]University of Michigan, Ann Arbor, Michigan; [4]Genentech Inc., South San Francisco, CA*

TP 766 **A Tailored Data Handling Workflow for Metabolite Profiling of Single Cells**; Felix Friedrich[1]; Cátia Marques[1]; Ingela Lanekoff[1]; *[1]Department of Chemistry — BMC, Uppsala University, Uppsala, Sweden*

TP 767 **Optimizing sample substrates for single-cell metabolomics analysis**; Eszter Szombati[1]; Ingela Lanekoff[1]; *[1]Department of Chemistry — BMC, Uppsala University, Uppsala, Sweden*

TP 768 **Unveiling Cellular Secrets: Mass Spectrometry Based Single-Cell Proteomic Analysis of Tissue samples from Familial Adenomatous Polyposis**; Ruiqi Jian[1]; Lihua Jiang[1]; Chenchen Zhu[1]; Tiffany Trinh[1]; Michael P. Snyder[1]; *[1]Department of Genetics, Stanford University School of Medicine, Stanford, CA*

TP 769 **Evotip meets the Uno – a transfer-free single cell proteomics approach**; Sibylle Pfammatter[1]; Rafaela Truffer[2]; Ralph Schlapbach[1]; Paolo Nanni[1]; *[1]Functional Genomics Center Zurich ETHZ/UZH, Zürich, Switzerland; [2]TECAN Group, Männedorf, Switzerland*

TP 770 **Live single cell mass spectrometry integration with Raman spectroscopy for drug screening**; Congrou Zhang[1]; Arno Germond[2]; Sylvia Le Dévédec[1]; Thomas Hankemeier[1]; Ahmed Ali[1]; *[1]Leiden Academic Centre for Drug Research, Leiden University, Leiden, Netherlands; [2]INRAE Centre Clermont-Auvergne-Rhône-Alpes, St Genès Champanelle, France*

TP 771 **Scalable Sample Preparation Workflow for Single Cell Proteomics**; Jing Wang[1]; Olanrewaju Awoyemi[1]; Herbi Yuliantoro[1]; Stephen J Valentine[1]; Peng Li[1]; *[1]West Virginia University, Morgantown, WV*

TP 772 **Two-Dimensional Nanoflow Liquid Chromatography Platform for Deep Single-Cell Proteomics**; Madi Johnston[1]; Xiaofeng Xie[1]; Kei Webber[1]; Siqi Huang[1]; Thy Truong[1]; Ryan T. Kelly[1]; *[1]Brigham Young University, Provo*

TP 773 **Towards top-down proteomic analysis of limited samples and single cells using porous layer open tubular columns**; Michal Gregus[1]; Yunfan Gao[1]; Anne-Lise Marie[1]; Somak Ray[1]; Alexander R. Ivanov[1]; *[1]Northeastern University, Boston, MA*

TP 774 **Enhancing Sensitivity and Throughput for Low-Input Proteomics: Impact of Tip Integration, Column Length, and Sub-50 µm Internal Diameter Columns**; Thy Truong[1, 2]; Siqi Huang[1]; Xiaofeng Xie[1, 2]; Ryan T. Kelly[1, 2]; *[1]Brigham Young University, Provo, UT; [2]MicrOmics Technologies, Spanish Fork, UT*

TP 775 **Single-cell Exploration of Drosophila Oogenesis Identifies Key Actin Regulators**; Merin M Rixen[1]; Joseph A. Loo[2]; Margot E Quinlan[3]; Rachel Loo[2]; *[1]UCLA, Los Angeles, CA; [2]UCLA, Los Angeles; [3]UCLA, Los Angeles, California*

TP 776 **Automated Single Cell Lipidomics for Mapping MSC Heterogeneity**; Alexandria R Van Grouw[1]; Samuel M Erlich[1]; Alexandre E Dunnum[1]; Joseph L Corstvet[1]; Samuel G. Moore[1]; Johnna S Temenoff[1]; Craig R Forest[1]; Facundo M Fernández[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

TP 777 **High-efficiency dual-LIT miniature mass spectrometer enables single-cell lipidomics at high structural specificity**; Zhijun Cai[1]; Ningxi Li[1]; Siming Cheng[1]; Xiaoxiao Ma[1]; Zheng Ouyang[1]; *[1]Tsinghua, Beijing, China*

TP 778 **The Good and The Bad of Single-Cell Proteomics by the Most Sensitive Mass Spectrometers - Early Mouse Embryos as Example**; Mo Hu[1]; Yuan Yuan[2]; Yinghui Zheng[2]; Xiaoliang Sunney Xie[1, 2]; *[1]Beijing Changping Laboratory, Beijing, China; [2]Peking University, Beijing, China*

TP 779 **Significant impact of laboratory consumable surfaces and sample preparation buffer composition for low-cell number or single-cell proteomics**; Christopher Kune[1]; Sylvia Tielens[2]; Maximillien Fléron[3]; Dominique Baiwir[3]; Denis Vandormael[4]; Laurent Nguyen[2]; Gauthier Eppe[1]; Gabriel Mazzucchelli[1, 3]; *[1]Mass Spectrometry Laboratory, MolSys Research Unit, University of Liege, Liege, Belgium; [2]Laboratory of Molecular Regulation of Neurogenesis, GIGA-Stem Cells, University of Liège, Liège, Belgium; [3]GIGA Proteomics Facility, University of Liège, Liège, Belgium; [4]Sirris, Liege, Belgium*

TP 780 **Single-cell metabolomics and lipidomics reveal increased diversity and sub-populations in senescent cells**; Catia Marques[1]; Felix Friedrich[1]; Francesca Castoldi[2];

Federico Pietrocola[2]; Ingela Lanekoff[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Karolinska Institutet, Solna, Sweden*

TP 781 **Liquid chromatography coupled to untargeted lipidomics of single-cells with fluorescent live cell imaging of lipid droplets**; Johanna Von Gerichten[1]; Kyle D.G. Saunders[1]; Anthony D. Whetton[2]; Melanie Bailey[1]; *[1]University of Surrey, School of Chemistry and Chemical Engineering, Guildford, United Kingdom; [2]vHive, School of Veterinary Medicine, School of Biosciences and Medicine, University of Surrey, Guildford, United Kingdom*

TP 782 **Novel Nanoliter-Volume Sample Injection Technique Enables Top-down Proteomic and N-glycomics CE-MS-Based Profiling of Single Cells**; Yunfan Gao[1]; Michal Gregus[1]; Anne-Lise Marie[1]; Alexander R. Ivanov[1]; *[1]Northeastern University, Boston, MA*

TP 783 **An open source autosampler for trace proteomics of tissue samples**; Nathaniel B Axtell[1]; Kei Webber[1]; Siqi Huang[1]; Tarah Gudmundson[1]; Ryan T Kelly[1]; *[1]BYU, Provo, UT*

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TP 784 **Explanation for Discrepancies in Quantitative Mass Spectrometric Analysis of RNA Modifications**; Frank Morales Shnaider; *university of north carolina greensboro, Greensboro, NC*

TP 785 **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[1]; Karyn D. Howard[1]; Michael J. Myers[1]; *[1]FDA/CVM, Laurel, MD*

TP 786 **Development of a sensitive and high-throughput UPLC–MS/MS method for the quantification of multiple antiretrovirals in human tissues**; Raymond E. West III[1]; Patrick J. Oberly[1]; Thomas D. Nolin[1]; Aaron S. Devanathan[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

TP 787 **Development and Validation of a Simple and Rugged LC-MS/MS Method to Measure Amifampridine and N-Acetyl-Amifampridine in Human Plasma**; Nick Peng[1]; Jayce Brown[1]; Ardeshir Khadang[1]; *[1]Axis Clinicals, Dilworth, MN*

TP 788 **Characterization of new psychoactive substances using high resolution mass spectrometry structural assignment software**; Alan Barnes[1]; Peter Schein[2]; David I Dixon[3]; Molly F Millea[3]; Emily G Armitage[1]; Ben Barrett[4]; Ryan E Mewis[3]; Oliver B Sutcliffe[3]; Neil J Loftus[1]; *[1]Shimadzu Corporation, Manchester, United Kingdom; [2]Shimadzu Deutschland GmbH, Duisburg, Germany; [3]MANchester DRug Analysis and Knowledge Exchange (MANDRAKE), Manchester Metropolitan University, Manchester, United Kingdom; [4]Shimadzu UK Limited, Milton Keynes, United Kingdom*

TP 789 **Development of Highly Sensitive Bioanalytical Methods for Peptide Based Therapeutics**; Xiaodong Zhu[1]; Steven Hoehne[1]; Jingguo Hou[1]; Xiaomei Bian[1]; Leimin Fan[1]; *[1]Worldwide Clinical Trials, Austin, TX*

TP 790 **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[1]; Melissa Mofikoya[2]; *[1]Thermo Fisher Scientific Inc, Madison, WI; [2]Thermo Fisher Scientific Inc., Madison, WI*

TP 791 **Analysis of Ibuprofen and Three Modulator Drugs of Cystic Fibrosis Triple Combination Therapy in Human Plasma by LC-MS/MS**; Xiaolin Li[1]; Daniela M. Schlatzer[1]; Tracey L. Bonfield[1]; Mark R. Chance[2]; *[1]Case Western Reserve University, Cleveland, OH; [2]Case Western Reserve University, Cleveland, Ohio*

TP 792 **Comprehensive characterization of phytosiderophore-metal complexes with LC-QTOFMS and IM-MS**; Andreea Spiridon[1]; Eva Oburger[1]; Tim Causon[1]; Stephan Hann[1]; *[1]University of Natural Resources and Life Sciences, Vienna, Vienna, Austria*

TP 793 **Sensitive and selective quantitation of bimatoprost in human plasma using accurate mass spectrometry**; Ian Moore[1]; Sujata Rajan[2]; Rahul Baghla[3]; Eshani Galermo[3]; *[1]SCIEX, Framingham; [2]SCIEX, Bangalore, India; [3]SCIEX, Redwood City, CA*

TP 794 **Redefining bioanalysis: assessment of a mass spectrometer robustness versus complex matrix**; Elliott Jones[1]; Rahul Baghla[1]; Ebru Selen[1]; Ian Moore[2]; Eshani Galermo[1]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Framingham*

TP 795 **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[1]; Dan Li[1]; Yangzhen Zheng[1]; Jinlian Lu[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

TP 796 **Sensitive quantitative LC-MS/MS method of steroid hormones determination in adipose tissue as a helpful tool in obesity research**; Rafal Szewczyk[1, 2]; Anna Lenartowicz[1]; Alina Kuryłowicz[3]; Katarzyna Krupczyńska-Stopa[1, 2]; Maciej Stopa[1, 2]; *[1]LabExperts sp z o.o., Gdańsk, Poland; [2]Bioanalytic sp z o.o., Gdańsk, Poland; [3]Department of Human Epigenetics, Mossakowski Medical Research Centre, Polish Academy of Sciences, Warsaw, Poland*

TP 797 **A Novel Microliter Volume Injection System Based on the High Contact Angle Pinning Phenomena for High-Throughput MS**; Nate Hoxie[1]; Jenna Miller[1]; Vijay Veerisetty[1]; Meghav Verma[1]; John Janiszewski[1]; Jonathan Shrimp[1]; Bolormaa Baljinnyam[1]; Michael Ronzetti[1]; Peter Kovarik[2]; Tom Covey[2]; Chang Liu[2]; Richard B van Breemen[3]; Gary J Van Berkel[4]; Sam Michael[1]; Anton Simeonov[1]; Matthew D Hall[1]; Savannah Wood[1]; *[1]National Center for Advancing Translational Sciences, NIH, Rockville, MD; [2]SCIEX, Concord, ON; [3]Linus Pauling Institute, Oregon State University, Corvallis, OR; [4]Van Berkel Ventures, LLC., Oak Ridge, TN*

TP 798 **A UHPLC-HRMS method to record cyanotoxins and related secondary metabolites: A case study in Lake Stechlin (Ger)**; Janine F. M. Otto[1, 2]; Christine Kiel[3]; Jens C. Nejstgaard[3]; Georg Pohnert[2]; Stella A. Berger[3]; Nico Ueberschaar[1]; *[1]Friedrich Schiller University Jena, Mass Spectrometry Platform, Jena, Germany; [2]Friedrich Schiller University Jena, Institute of Inorganic and Analytical Chemistry, Jena, Germany; [3]Leibniz Institute of Freshwater Ecology and Inland Fisheries, Stechlin, Germany*

TP 799 **UHPLC-tandem MS quantitation of Quorum Sensing molecules in plasma samples of patients with AKI (Acute Kidney Injury) in sub-intensive care**; Alex Africano[1]; Vito Fanelli[1]; Vincenzo Cantaluppi[2]; Claudio Medana[1]; Federica Dal Bello[1]; *[1]University of Turin, Torino, Italy; [2]University of Eastern Piedmont, Novara, Italy*

TP 800 **Toward a predictive model of the optimal supported liquid extraction (SLE) strategies for small molecule bioanalysis by LC-MS/MS**; Yuxiang Cui[1]; Xiaorong Liang[1]; Brian Dean[1]; Liuxi Chen[1]; *[1]Genentech Inc, South San Francisco, CA*

TP 801 **Simultaneous Quantitation and Discovery (SQUAD) Metabolomics Workflow on the Orbitrap IQ-X for the Analysis of Fecal Bile Acids**; Allison Stewart[1]; Bashar Amer[2]; Rahul Deshpande[1]; Andrew Percy[3]; Krista Backiel[3]; Joshua P. Kline[2]; Brandon Bills[2]; Susan Bird[2]; *[1]ThermoFisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Cambridge Isotope Laboratories, Tewksbury, Massachusetts*

TP 802 **Detection, quantification, and confirmation of 14 compounds affecting hypoxia-inducible factor in equine plasma and urine by LC-HRMS**; Matthew A. Adreance[1, 2]; Fuyu Guan[1, 2]; Savannah Fay[1, 2]; Mary A. Robinson[1, 2]; *[1]Department of Clinical Studies – New Bolton Center , School of Veterinary Medicine, University of Pennsylvania, Kennett Square, PA; [2]Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA*

TP 803 **Quantification of Sirolimus in Equine Whole Blood by UHPLC-MS/MS**; Jaclyn R. Missanelli[1, 2]; Youwen You[1, 2]; Rachel M. Proctor[1, 2]; Andrew Van Eps[1]; Joanne Haughan[1];

Mary A. Robinson[1, 2]; *[1]University of Pennsylvania School of Veterinary Medicine, Pennsylvania, PA; [2]Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA*

TP 804 **Rapid and Sensitive detection of enantiomeric D- and L-Lactae in cancer cell Using High-performance Liquid Chromatography-Negative Electrospray Mass Spectrometry**; Liangqiao Bian[1]; Raj Ritu[2]; Eul Hyun Suh[2]; *[1]SCAAC, UT Arlington, Arlington, TX; [2]Department of Pharmaceutical Sciences, UNT System College of Pharmacy, University of North Texas Health Science Center, Fort Worth, TX*

TP 805 **Rapid, Sensitive and Direct Quantitation of Tiotropium at sub-pg/mL in Plasma using Shimadzu LCMS-8060NX**; Yogesh G Arote[1]; Avinash B Gaikwad[1]; Chaitanya Krishna A[1]; *[1]ADC-Shimadzu Analytical India Pvt Ltd, NAVI MUMBAI, India*

STABLE ISOTOPE LABELING
806-820

TP 806 **SLC45A4 encodes a mitochondrial transporter that promotes GABA synthesis from ornithine**; Cecilia Colson[1]; James Atherton[1]; Yujue Wang[1]; Xiaoyang Su[1]; *[1]Rutgers University- New Brunsw, New Brunswick, NJ*

TP 807 **Monitoring de novo Biosynthesis of Amino Acids with 13C-labeled Glucose**; Simpson Jeffrey[1]; Eric M George[2]; Greenwalt Scott[1]; Heather Platt[1]; Suresh Annangudi[1]; *[1]Corteva Agriscience, Indianapolis, IN; [2]Purdue University, West Lafayette, IN*

TP 808 **ClickZip: ultra-stable lanthanide mass tags for multiplex assay**; Tomáš David[1]; Miroslava Šedinová[1]; Aneta Myšková[1, 2]; Ibrahim Demirci[1]; Jiří Böserle[1]; Helena Mertlíková Kaiserová[1]; Miroslava Litecká[3]; Blanka Klepetářová[1]; Karel Čížek[1]; Lenka Maletínská[1]; Miloslav Polasek[1]; *[1]Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic; [2]University of Chemistry and Technology Prague, Prague, Czech Republic; [3]Institute of Inorganic Chemistry of the CAS, Husinec-Řež, Czech Republic*

TP 809 **Metabolomic comparison between hepatic fibrosis and pulmonary fibrosis using 13C-MFA(Metabolic Flux Analysis)**; Mi Jeong Kim[1]; Ha Eun SONG[1]; Hyun Ju Yoo[1]; *[1]ASAN Medical center, SEOUL, South Korea*

TP 810 **Discovering mode of action of novel compounds through nascent proteome analysis: Bostrycin induces cell death via ferroptotic pathways**; Lina-Marie Wagner[1]; Syed A. Ali[1]; Isabelle Becher[2]; Mira Burtscher[2]; Mikhail Savitski[2]; Jeroen Krijgsveld[1, 3]; *[1]German Cancer Research Center, Heidelberg, Germany; [2]EMBL, Heidelberg, Germany; [3]Heidelberg University, Medical Faculty, Heidelberg, Germany*

TP 811 **14-plex DeAla Isobaric Reagents for High-Throughput Proteome-wide Quantification**; Peng-Kai Liu[1]; Ting-Jia Gu[2]; Danqing Wang[3]; Lingjun Li[1, 2, 3]; *[1]Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

TP 812 **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[1]; Alban J Allentoff[1]; Sharon X Gong[1]; Samuel Bonacorsi, Jr. [1]; Jim X Shen[1]; Felicia Dunsmuir[2]; Daniel Bennett[2]; *[1]Bristol Myers Squibb, Princeton, NJ; [2]Syneos Health, Somerset, New Jersey*

TP 813 **Application of tandem mass tag labeling to understand virus resistance to free chlorine**; Chonglin Zhu[1]; Yinyin Ye[1]; *[1]University at Buffalo, Buffalo, NY*

TP 814 **Metabolic pulse-chase multiplex proteomics reveals impaired protein turnover in aging brain is due to reduced turnover of proteolytic proteasome subunits**; Jeffrey N Savas[1]; Nalini R. Rao[2]; Arun Upadhyay[2]; *[1]Northwestern University, Feinberg School of Medicine, Chicago, IL; [2]Northwestern University Feinberg School of Medicine, Chicago, IL*

TP 815 **Stable Isotope Resolved Metabolomics of cancer cells by Cation-Exchange Ion Chromatography Coupled to Ultra-High Resolution Mass Spectrometry**; Mohamed M. Y. Kaddah[1]; Teresa Fan[1]; Andrew Lane[1]; Richard Higashi[1]; *[1]University of Kentucky, Lexington, KY*

TP 816 **24-plex high throughput quantitation of carboxylic acid metabolites for pharmaceutical dose response curves.**; BRIANA Mwinkom TENGAN[1]; Micheal Armbruster[2]; James Edwards[2]; *[1]Saint Louis University, Saint Louis, MO; [2]SAINT LOUIS UNIVERSITY, St Louis, MO*

TP 817 **18O-water labelling enables protein turnover measurements in embryogenesis.**; Edward R Cruz[1]; Argit Marishta[1]; Alex Johnson[1]; Aleigha Reynolds[1]; Michael Neinast[1]; Joseph Crapse[1]; Joshua D. Rabinowitz[1]; Eric F. Wieschaus[1]; Martin Wuhr[1]; *[1]Princeton University, Princeton, NJ*

TP 818 **Analytical solution for dynamic label incorporation in atom-based metabolic labeling**; Henock Deberneh[1]; Rovshan Sadygov[2]; *[1]The University of Texas Medical Branch, Galveston, TX; [2]University of Texas Medical Branch, Galveston, TX*

TP 819 **A 23rd proteogenic amino acid? The Hidden Homoarginine Proteome Revealed Using a Novel Activity-based Arginylation Profiling Platform**; Daniel H Ramirez[1]; Zongtao Lin[1]; Benjamin A Garcia[1]; *[1]Washington University in St. Louis, St. Louis, MO*

TP 820 **A comprehensive protein turnover atlas for drug discovery**; Goetz Hagemann[1]; Barbara Schnitzer[1]; Leonie Reichert[1]; Alexander Betz[1]; Christin Zasada[1]; Hannes Hahne[1]; *[1]OmicScouts GmbH, Freising, Germany*

WEDNESDAY POSTERS

Set up all Wednesday posters
7:00 - 8:00 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
7:00 - 8:00 pm

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[1]; Austin Arias[1]; Mac Gilliland[1]; *[1]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[1]; Norman Ahlmann[2]; Juan F. García-Reyes[1]; Joachim Franzke[2]; *[1]University of Jaén, Jaén, Spain; [2]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[1]; Josie Daldegan Rezende[2]; Jace W. Jones[2]; *[1]MassTech Inc, Columbia, MD; [2]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[1]; Mengliang Zhang[1]; Ngee Sing Chong[1]; Victoria Bascou[1]; *[1]Middle Tennessee State University, Murfreesboro, TN*

WP 005 **Understanding Signal Enhancement of Lipids by Fluoride-Containing Additives in Electrospray Ionization**; Emerson Hernly[1]; Aiming Zheng[1]; Syeda Nazifa Wali[1]; Julia Laskin[1]; *[1]Purdue University, Department of Chemistry, West Lafayette, IN*

WP 006 **Ambient Gas Atmosphere Influence on Onset Potential for Electrospray Ionization Mass Spectrometry**; Khadija Khetabi[1]; Amy Le[1]; Andre R. Venter[2]; Richard B. Cole[1, 3]; *[1]Sorbonne Universite - Paris 06, Paris Cedex 05, France; [2]Western Michigan University, Kalamazoo, MI; [3]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[1]; Nelson Vinueza[1]; *[1]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[1]; Yu-Chie Chen[1]; *[1]National Yang Ming Chiao Tung University, Hsinchu City, Taiwan*

ANTIBODIES & ANTIBODY DRUG CONJUGATES I
009-039

WP 009 **Decoding mAb Charge Variants: Unveiling Hidden Complexity with Native CE-MS Analysis**; Weihan Wang[1]; Qing Mike Tang[1]; Ping Hu[1]; *[1]Janssen Research & Development, LLC, Malvern, PA*

WP 010 **An Integrated Strategy to Identify Tyrosine Sulfation/phosphorylation in Therapeutic Proteins**; Eunju Jang[1]; Fengfei Ma[2]; Daniela Tomazela[1]; Laurence Fayadat-Dilman[1]; Mohammad Ahmed Al-Sayah[2]; *[1]Protein Sciences, Discovery Biologics, Merck & Co., Inc., South San Francisco, CA, USA, South San Francisco, California; [2]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**; Benqian Wei[1]; Fengfei Ma[2]; Daniela Tomazela[3]; Laurence Fayadat-Dilman[3]; *[1]Analytical Research and Development, Merck & Co., Inc., Rahway, NJ; [2]Analytical Research and Development, Merck & Co., Inc., South San Francisco, CA; [3]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[1]; Elliott Jones[1]; Zoe Zhang[1]; *[1]SCIEX, Redwood City, CA*

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[1]; Ashley Yoon[1]; Edward J. Hsieh[1]; Magdeleine Hung[1]; Daniela M. Tomazela[1]; *[1]Gilead Sciences Inc., Foster City, CA*

WP 014 **Exposing distinctive quantitative traits in structural isomers on Fc-glycans of human IgG subclasses**; Weiwei Wang[1, 2]; Joshua Maliepaard[1, 2]; Gestur Vidarsson[1, 2]; Albert J.R. Heck[1, 2]; Karli Reiding[1, 2]; *[1]Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht University, Padualaan 8, 3584 CH, Utrecht, Netherlands; [2]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[1]; Alyssa Erlenbeck[1]; Hayden Fisher[2]; Isabel Elliot[2]; Mark S Cragg[2]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, Michigan; [2]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[1]; Xiaoxi Zhang[2]; Rafael Melani[3]; Eugen Damoc[1]; Kyle L. Fort[1]; Min Du[4]; Claire Dauly[1]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Thermo Fisher Scientific, Shanghai, China; [3]Thermo Fisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, Remote, MS*

WP 017 **Detailed characterization of monoclonal antibodies charge variants using capillary electrophoresis and tandem mass spetrometry**; Lola Alez-Martin[1, 2]; Pascal Houzé[2]; Rania Joomun[2]; Nathalie Mignet[2]; Yannis-Nicolas François[1]; Rabah Gahoual[2]; *[1]Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, Strasbourg, France; [2]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[1]; Teressa Nunez De Villavicencio Diaz[1]; Chelsea Reitzel[1]; Victoria Lange[1]; Minyoung Park[1]; Emma Beadle[1]; Lin Wu[1]; Marko Jovic[1]; Rosalin M. Dubois[1]; Amber L. Couzens[1]; Jin Duan[1]; Xiaobing Han[1]; Qixin Liu[1]; Bin Ma[1]; *[1]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[1]; Qing Ma[2]; Raymond Cha[2]; Kevin J Zemaitis[3]; Robin Difrancesco[2]; Gene D. Morse[2]; Troy D. Wood[1, 2]; *[1]SUNY at Buffalo, Buffalo, NY; [2]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; [3]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[1]; Mark Benhaim[1]; Nate Joh[1]; *[1]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[1]; Jim Zanghi[2]; Chang Liu[3]; Michael T Kim[3]; Cynthia Quan[3]; Keyang Xu[3]; *[1]Genentech, Inc., South San Francisco, CA; [2]Genentech Inc., South San Francisco, CA; [3]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[1]; Jeffrey J Liu[1]; Gang Xiao[1]; Aman Makaju[1]; Pavel V. Bondarenko[1]; *[1]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[1]; Hefeng Zhang[1]; Zhiyu Li[1]; Hongmei Wang[1]; Nan Zhao[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

WP 024 **Characterization of Coformulated Therapeutic Proteins by Mass Spectrometry**; Lidong He[1]; Qingchun Zhang[1]; Suminda Hapuarachchi[1]; *[1]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 developability assessments**; Esther Marie Martin[1]; Kyna Griffiths[1]; Noemi Mallorqui-Fernandez[1]; Stanislas Blein[1]; *[1]AstraZeneca, Cambridge, United Kingdom*

WP 026 **Size Exclusion Column Considerations for Antibody Drug Conjugates**; Alycia K Uyeoka[1]; Fan Zhang[1]; Esther Kofman[1]; Mehabaw Derebe[1]; Laurence Fayadat-Dilman[1]; Jason Hogan[1]; *[1]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[1]; Philip H Yoo[1]; Lana V Fabia[1]; Nicole A Schneck[1]; *[1]GSK, Collegeville, PA*

WP 028 **Sample preparation and nLC-MS/MS optimization for mAB characterizing**; Rodrigo S C Brant[1]; Kelly Cavalcanti Machado[2]; Thiago Bousquet Bandini[2]; Hulyana Brum[2]; Anna Erika Vieira De Araujo[1]; Iaralice Medeiros De Souza[1]; Michel Batista[2]; *[1]Fiocruz, Curitiba, Brazil; [2]Mass Spectrometry Facilty, Fiocruz, Curitiba, Brazil*

WP 029 **Development of a High-Throughput Host Cell Proteomics Method to Support Next Generation Manufacturing of Biopharmaceuticals**; Jake A. Melby[1]; Samik Das[1]; Ken Lee[1]; Wei Xu[1]; Yu Shi[1]; *[1]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[1]; Vadiraja B. Bhat[2]; Sunil Kumar[1]; Deepika Sarin[1]; *[1]Indian Institute of Technology Delhi, New Delhi, India; [2]Agilent technologies, Bangalore, India*

WP 031 **Localization and Quantification of Lysine Conjugation by Peptide Mapping**; Amber Peariso[1]; Zhongping Liao[1]; *[1]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[1]; Vincent Larraillet[2]; Sabrina Thalhauser[1]; Tobias Graf[1]; Manuel Endesfelder[2]; Stefanie Wohlrab[1]; *[1]Roche Diagnostics GmbH, Penzberg, Germany; [2]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[1]; Eva Vosika[2]; Juergen Fichtl[2]; Marco Boettger[3]; Vincent Larraillet[3]; *[1]ProteinMetrics LLC, Cupertino, CA; [2]Roche Technical Development, Roche Diagnostics GmbH, Penzberg, Germany; [3]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[1]; Bradley Prater[2]; Ying Qing Yu[3]; Mark Wrona[3]; Nick Pittman[4]; Guillaume Bechade[4]; Scott Berger[3]; *[1]Waters Corporation, Milford, MA; [2]Similis Bio, Sunnyvale, CA; [3]Waters, Milford, MA; [4]Waters Corporation, Wilmslow, United Kingdom*

WP 035 **Complete Characterization of Trastuzumab Deruxtecan, a Cysteine-linked antibody drug conjugate, using high resolution accurate mass (HRAM) Mass Spectrometry**; Xiaoxi Zhang[1]; Min Du[2]; *[1]ThermoFisher Scientific, Shanghai, China; [2]Thermo Fisher Scientific, Lexington, MA*

WP 036 **Rapid Quality Assessment of Therapeutic Monoclonal Antibodies through Automated Middle-level Mass Spectrometry**; Andreas Naegeli[1]; Olle De Bruin[2]; Phil Widdowson[1]; Camilla Sivertsson[3]; Gunilla Larsson[2]; Rolf Lood[1]; *[1]Genovis AB, Kävlinge, Sweden; [2]BioInvent International AB, Lund, Sweden; [3]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[1]; Weijing Liu[2]; Xuepu Li[3]; Min Du[4]; *[1]ThermoFisher Scientific, Shanghai, China; [2]ThermoFisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Shanghai, China; [4]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[1, 2]; Ioannis Karageorgos[1, 2]; Trina Mouchahoir[1, 2]; Zvi Kelman[1, 2]; John Schiel[1, 2]; John Marino[1, 2]; *[1]National Institute for Standards and Technology, Gaithersburg, MD; [2]Institute for Bioscience and Biotechnology Researc, Rockville, MD*

ARTIFICIAL INTELLIGENCE IN MS INSTRUMENTATION AND APPLICATIONS I

040-065

WP 040 **Machine Learning-Guided Exploration of Known and Unknown Chlorinated Disinfection Byproducts in Nontargeted Mass Spectrometry Analysis**; Tingting Zhao[1]; Nicholas J. P. Wawryk[2]; Shipei Xing[1]; Brian Low[1]; Huaxu Yu[1]; Yukai Wang[1]; Qiming Shen[2]; Xing-Fang Li[2]; Tao Huan[1]; *[1]University of British Columbia, Vancouver, BC; [2]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[1]; Léa LEDOUX[1]; Pierre Tirilly[2]; Bertrand Meresse[3]; Claude Alain Maurage[4]; Marie Duhamel[1]; Isabelle Fournier[1]; Michel Salzet[1]; *[1]PRISM - Inserm U1192, Villeneuve d'Ascq Cedex France, France; [2]UMR 9189 Cristal, Villeneuve d'ascq, France; [3]Institute for Translational Research in Inflammation, Villeneuve d'Ascq Cedex France, France; [4]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[1]; Fabien Fontaine[1]; Luca Morettoni[2]; Ismael Zamora[1]; *[1]Mass Analytica, S.L, Sant Cugat del Vallés, Spain; [2]Mass Analytica, S.L, Bettona, Italy*

WP 043 **Towards automated development of charged particle optical instrumentation using a novel optimization framework**; Kilian Huber[1, 2]; Tom Wirtz[1]; Quang Hung Hoang[1]; *[1]Luxembourg Institute of Science and Technology, Belvaux, Luxembourg; [2]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[1]; Matthew Turner[1]; Luke Durell[1]; Sean Colby[1]; Sydney Schwartz[1]; Charles Doll[1]; Eva Brayfindley[1]; Fanny Chu[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

WP 045 **DiProQ: A Deep Learning-Driven Method for Differential Analysis in Quantitative Proteomics**; Hojin Yoo[1]; Jose Cruz Castelo[1]; Namgil Lee[1, 2]; Heejung Yang[1, 3]; *[1]Bionsight Inc, Chuncheon-si, South Korea; [2]Department of Information Statistics, Kangwon National University,, Chuncheon-si, South Korea; [3]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[1]; Joel Lapin[2]; Mathias Wilhelm[2]; Lukas Käll[1]; *[1]KTH Royal Institute of Techonology, Stockholm, Sweden; [2]Technical University of Munich, Freising, Germany*

WP 047 **Revolutionizing Proteomics: Ultra-Fast, High-Accuracy Peptide Sequencing with Enhanced GraphNovo Algorithm**; Zeping Mao[1]; Lei Xin[2]; Shengying Pan[2]; Baozhen Shan[2]; *[1]University of Waterloo, Waterloo, ON; [2]Bioinformatics Solutions Inc., Waterloo, ON*

WP 048 **A multidimensional data analysis approach for clinical analysis by mass spectrometry**; Haoyue Zhang[1]; Wenpeng Zhang[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China*

WP 049 **Tackling mass degeneracy in mass mapping and sequence analysis of nucleic acids**; Daniele Fabris[1]; Daniele Rollo[1]; Thomas Kenderedine[1]; *[1]University of Connecticut, Storrs, CT*

WP 050 **Integrating Data Science in MS: Insights into MS/MS Fragmentation and Differential Mass Spectrometry Behaviour**; Stepan Stepanovic[1]; Gerard Hopfgartner[2]; *[1]University of Geneve, Olten, Switzerland; [2]University of Geneva, Geneva, Switzerland*

WP 051 **AI Guided Platform for Released Peptide Mapping Method Development Using a Transformer Model**; Mengxiao Liu[1]; Longyun Guo[1]; Bing Ran[1]; Xi Chen[1]; Moyin Zhou[1]; Tongdan Wang[1]; Jincui Huang[1]; *[1]WuXi Biologics, Shanghai, China*

WP 052 **∏-SPECFormer: Pretraining Improves SPectrum Embedding through Contrastive Learning with TransFormer**; Tianze Ling[1, 2]; Fan Xu[3]; Jun Xia[4]; Stan Z. Li[4]; Yu Wang[3]; Cheng Chang[2]; *[1]Tsinghua University, Beijing, China; [2]National Center for Protein Sciences (Beijing), Beijing, China; [3]Peng Cheng Laboratory, Shenzhen, China; [4]Westlake University, Hangzhou, China*

WP 053 **DeepiRT: Incorporating chromatography information boosts performance of iRT prediction model**; Alexandros Pachos[1]; Sandra Schär[1]; Arthur Viode[1]; An-phi Nguyen[1]; George Rosenberger[1, 2]; Oliver M. Bernhardt[1]; Roland Bruderer[1]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Zurich, Switzerland; [2]Bruker Switzerland AG, Faellanden, Switzerland*

WP 054 **Enhancing AlphaFold2 Protein Structure Prediction Using Tandem Mass Spectrometry**; Seonggwang Jeon[1]; Eunok Paek[1]; *[1]Hanyang University, Seoul, South Korea*

WP 055 **Machine and Deep Learning Classification of Bacterial Species using Two-Dimensional Tandem Mass Spectrometry**; L. Edwin Gonzalez[1]; Dalton T Snyder[2]; Harman Casey[2]; Yanyang Hu[1]; Joseph V. Caruso[1]; Megan Guetzloff[2]; Nicole Huckaby[2]; Eric T Dziekonski[1]; R. Graham Cooks[1]; *[1]Purdue University, Department of Chemistry, West Lafayette, IN; [2]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 **Orthrus: a hybrid, AI-powered, and cloud-ready peptide sequencing pipeline on Google Colab**; Yun Chiang[1, 2]; Matthew Collins[1, 3]; *[1]University of Copenhagen, Copenhagen, Denmark; [2]Université Côte d'Azur, Nice, France; [3]University of Cambridge, Cambridge, United Kingdom*

WP 058 **Benchmarking of a machine learning model developed for quantitative metabolomics**; Jeff Pruyne[1]; Joshua D. Lauterbach[1]; Ana S.H. Costa[1]; Devesh Shah[1]; Jack Howland[1]; Luke S Ferro[1]; Timothy Kassis[1]; Mimoun Cadosch Delmar[1]; Jennifer M Campbell[1]; *[1]Matterworks, Inc., Somerville, MA*

WP 059 **Towards Science Autonomy for Planetary Missions: Application to Mass Spectrometers for Future Missions**

to Mars, Titan, and Ocean Worlds; Victoria Da Poian[1, 2]; Eric Lyness[1, 2]; Desmond A. Kaplan[1, 3]; Ryan M. Danell[1, 4]; William B Brinckerhoff[1]; Melissa Trainer[1]; Xiang Li[1]; Andrej Grubisic[1]; Friso H.W. Van Amerom[1]; *[1]NASA Goddard Space Flight Center, Greenbelt, MD; [2]Microtel LLC, Greenbelt, MD; [3]KapScience LLC, Tewksbury, MA; [4]Danell Consulting, Inc., Winterville, NC*

WP 060 **MS-KGbot: A Conversational AI-Agent for Accessible Mass Spectrometry Metabolomics Data Mining**; Emma Tysinger[1, 2]; Lucas Pradi[2]; Madina Bekbergenova[2, 3]; Benjamin Navet[3]; Olivier Kirchhoffer[4]; Florence Mehl[5]; Marco Pagni[5]; Jean-Luc Wolfender[4]; Fabien Gandon[6]; Louis Felix Nothias[2, 3]; *[1]MIT, Cambridge, MA; [2]Université Côte d'Azur, CNRS, ICN, Nice, France; [3]Interdisciplinary Institute for Artificial Intelligence (3iA) Côte d'Azur, Nice, France; [4]School of Pharmaceutical Sciences, University of Geneva, Geneva, Switzerland; [5]Swiss Institute of Bioinformatics (SIB), Lausanne, Switzerland; [6]INRIA, Université Côte d'Azur, CNRS, I3S, Sophia-Antipolis, France*

WP 061 **End-to-end MRM Quantification with Deep Learning Networks**; Mihira Kasun[1]; Pasindu Tennakoon[1]; Rukshan Wijesinghe[1]; Leiver Campeon[1]; Lalin Theverapperuma[1]; Andi Krupke[1]; *[1]Expert Intelligence, Santa Clara, CA*

WP 062 **Prediction of ‘unspecific’ peptide products: enhancing the use of broad-specificity enzymes for mapping of post-translational modifications**; Xuehui Jiang[1]; Victor Spicer[1]; Darien Yeung[1, 2]; Ying Lao[1]; Oleg Krokhin[1, 2, 3]; Rene Peiman Zahedi[1, 2, 3, 4]; *[1]Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; [2]Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; [3]Department of Internal Medicine, University of Manitoba, Winnipeg, MB; [4]Paul Albrechtsen Research Institute, Cancer Care Manitoba, Winnipeg, MB*

WP 063 **Nested Machine Learning Pipeline for Precision Targeted Mass Spectrometry**; Jia Fan[1]; Duran Bao[1]; Bo Ning[1]; Tony Hu[1]; *[1]Tulane University, New Orleans, LA*

WP 064 **Using Deep Learning for Spectra Translation between Ionization Modalities**; Frederick Zhang[1]; Michael Strobel[2]; Liping Liu[1]; Mingxun Wang[2]; Soha Hassoun[1]; *[1]Tufts University, Medford, MA; [2]University of California, Riverside, Riverside, CA*

WP 065 **Super-resolution: what is the best in time with genetic algorithm or in frequency with Artificial Intelligence for Fourier Transform MS?**; Léo CHENEAU[1]; Marc Haegelin[2]; Azad KICHIBAYOV[3]; Anna LEONTEVA[1]; Ulviyya ABDULKARIMOVA[3]; Pierre COLLET[1]; Christian Rolando[2]; *[1]Université de Strasbourg, Strasbourg, France; [2]Univ. de Lille, Sciences et Technologies, Villeneuve D'ascq, France; [3]UFAZ - French-Azerbaijani University, Baku, Azerbaijan*

BIOMARKERS: DISCOVERY I
066-102

WP 066 **Proteomic analysis of synovial lavage from patients with shoulder instability offers periostin as a molecular indicator for anterior shoulder instability**; Elizabeth Yohannes[1]; Rachel Milam[2]; Brendan Patterson[3]; James V. Nepola[3]; Joseph A. Buckwalter IV3[3]; Brian Wolf[3]; Felicity Say[2]; Katherine E. Free[1]; Joseph W. Galvin[2]; *[1]Department of Clinical Investigation, Madigan Army Medical Center, Tacoma, WA; [2]Department of Orthopaedic Surgery, Madigan Army Center, Tacoma, WA; [3]Department of Orthopaedic Surgery and Rehabilitation, University of Iowa, Iowa City, IA*

WP 067 **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[1]; Danielle Whitham[1]; Lilian Corrice[1]; Brian T. Pentecost[1, 2]; Kathleen F. Arcaro[2]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]University of Massachusetts Amherst, Amherst, MA*

WP 068 **A comprehensive analysis of serum from women with breast cancer and age-matched controls to determine candidate protein biomarkers**; Danielle Whitham[1]; Pathea S. Bruno[1]; Brian T. Pentecost[1]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY*

WP 069 **(H)Ear Me Out: Utilization of Earwax for the Identification of Chemical Markers of Ménière's Disease**; Allix M. Coon[1]; Gavin Setzen[2]; Rabi A. Musah[1]; *[1]University at Albany, State University of New York, Albany, NY; [2]Albany ENT & Allergy Services, Albany, NY*

WP 070 **Plasma Metabolomic and Proteomic Profiling of Anxious Dogs by HPLC-MS/MS: A Case-Control Study**; Claudia Gaither[1]; Robert Popp[2]; Francis Beaudry[1]; Christoph H Borchers[3]; Marion Desmarchelier[1]; *[1]Université de Montréal Saint-Hyacinthe Campus, Saint-Hyacinthe, QC; [2]MRM Proteomics Inc, Montreal, QC; [3]McGill University, Montreal, QC*

WP 071 **Ultra-deep profiling of human and rodent tissues allows for deepest ever analysis of protein expression levels**; Sandra Schär[1]; Jan Muntel[1]; Marco Tognetti[1]; Christopher Below[1]; Matevsz Stefancic[1]; Igor Sobanski[1]; Roland Bruderer[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

WP 072 **Proteomics Analysis for Prognosis Biomarkers Clear cell renal carcinoma Patients Undergoing Immunotherapy**; Virginia Campos Silvestrini[1]; Aline Gomes De Souza[1, 2]; Letícia Andrade Costa[1]; Sabrina Baroni[1, 2]; Ana Paula Masson[1]; André Aparecido da Silva Teles[1]; Denise Aparecida Zampieri[3]; Beatriz Boleta Fernandes[3]; José Lopes Bueno Junior[2, 3]; Alexandre Todorovic Fabro[3]; André Schmidt[3]; Fernanda Maria Peria[3]; Fernanda Cristina Gonçalves de Oliveira[3]; Liane Rapatoni[3]; Alison Luis Eburneo Pereira[2]; Olga Laura Sena Almeida[3]; Margaret Castro[3]; Matheus de Aquino Moreira Guimaraes[3]; Rodolfo Borges dos Reis[3]; Valdair Francisco Mugli[3]; Vitor Marcel Faça[1, 2]; Leandro Machado Colli[1, 2, 3]; *[1]Medical School of Ribeirao Preto - University of São Paulo, Ribeirao Preto, Brazil; [2]Blood center of Ribeirão Preto, Ribeirão Preto, Brazil; [3]University Hospital of Ribeirao Preto, Ribeirão Preto, Brazil*

WP 073 **Characterization of O-Glycan Profiles of IgA in Ankylosing Spondylitis: A New Approach for Primary and Secondary IgA Nephropathy Differentiation**; Hui-Ling Chiang[1]; Ming-Chi Lu[1, 2]; Ning-Sheng Lai[1]; Chien-Hsueh Tung[1]; Chih-Chia Yu[2]; *[1]Division of Immunology, Allergy and Rheumatology, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan; [2]Department of Medical Research, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan*

WP 074 **Pathogenic and Non-pathogenic E. colistrains Discrimination in Urine Samples by LC – IM – MS/MS and Machine Learning**; OROBOLA E. OLAJIDE[1]; Micheal Zirpoli[1]; Jingyi Zheng[1]; Ahmed M. Hamid[1]; *[1]Auburn University, AUBURN, AL*

WP 075 **Metabolomics of in vitro skin models: an aging study**; Abigale S Mikolitis[1, 2]; CDT Kye Yu[3]; Ethan M. McBride[1, 2]; Erick S. LeBrun[1, 2]; Zachary J. Sasiene[1, 2]; Mary Donnelly[1, 2]; Emilio S. Rivera[1, 2]; Jennifer Harris[4]; Mohamed Omar Ishak[5]; Emilia A. Solomon[2]; Claire K. Sanders[6, 7]; COL Chi Nguyen[3]; Francisca E. Rodriguez[1, 2]; Trevor G. Glaros[1, 2]; Phillip M. Mach[1, 2]; *[1]Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [2]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [3]United States Military Academy, West Point, NY; [4]Physical Chemistry and Applied Spectroscopy, Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM; [5]Transition to Operations/Readiness, Program Project Interface, Los Alamos National Laboratory, Los Alamos, NM; [6]Los Alamos National Laboratory, Los Alamos, NM; [7]Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM*

WP 076 **Discovery of Patient’s Specific Biomarker: Concept and Evaluation of a New Diagnosis Strategy**; Bertrand Rochat[1]; Jachen Barblan[2]; *[1]Université de Lausanne, Lausanne, Switzerland; [2]Université de Lausanne, Lausanne, Switzerland*

WP 077 **Investigation of idiopathic pulmonary fibrosis pathogenesis by multiple omics approaches**; Fei Wang[1];

Liang Jin[1]; Xue Wang[1]; Baoliang Cui[1]; Jan Schejbal[1]; Erik Hagendorn[1]; Yingli Yang[1]; Lori Duggan[1]; Lucy Phillips[1]; Annette Schwartz[1]; Neha Chaudhary[2]; Sarah Lloyd[3]; Yupeng (David) He[3]; Bhupinder Bawa[3]; Yu Tian[1]; *[1]AbbVie Bioresearch Center, Worcester; [2]AbbVie Cambridge Research Center, Cambridge, MA; [3]AbbVie Inc., North Chicago, IL*

WP 078 **In-depth Analysis of Plasma Proteomics: Are We Enriching Extracellular Vesicles, Platelets, or Soluble Proteins?**; Chiara Guerrera[1]; Cerina Chhuon[1]; Sara Ceccacci[1]; Ines Metatla[1]; Kevin Roger[1]; *[1]Necker Proteomics Platform, INSERM US24, Paris, France*

WP 079 **Bladder Cancer Biomarkers Analysis from Methanol Extracts from Pathology Specimens and Urine using LC-MS/MS**; Alexandra Izydorczak[1]; Wilfrido D. Mojica[1]; Troy D. Wood[1]; *[1]SUNY at Buffalo, Buffalo, NY*

WP 080 **Analyzing the Urinary Peptidome to Predict Neurogenic Bladder Risk in Spina Bifida Patients**; Hossein Fazelinia[1]; Hua Ding[1]; Deanne M Taylor[1]; Lynn A Spruce[1]; Jennifer Roof[1]; Dana Weiss[1]; Joanna Fesi[1]; Harry Ischiropoulos[1]; Stephen Zderic[1]; *[1]Children's Hospital of Philadelphia, Philadelphia, PA*

WP 081 **Proteomic Characterization of Extracellular Vesicles Purified by Dialysis Membrane Concentration and Electrophoresis as Compared to Standard Ultracentrifugation Techniques**; Nancy Henin[1]; Kenzie Rushing[2]; Katherine Moutis[1]; James N. Higginbotham[3]; Jeffrey L. Franklin[3]; Robert J. Coffey[3]; Amy-Joan L. Ham[1]; *[1]Belmont University, College of Pharmacy and Health Sciences, Nashville, TN; [2]Belmont University, College of Science and Math, Nashville, TN; [3]Vanderbilt University Medical Center, Nashville, TN*

WP 082 **Discovery of the serum peptidomic biomarkers related to gestational diabetes mellitus using LC MS/MS coupled with magnetic solid phase extraction**; Xi Gao[1, 2]; Guixue Hou[2]; Qunjie Wang[3]; Liang Lin[2]; Jin Zi[2]; Siqi Liu[1, 2]; *[1]University of Chinese Academy of Sciences, Beijing, China; [2]BGI Genomics, ShenZhen, China; [3]Biosepur, Suzhou, China*

WP 083 **Development of an IP-MALDI Method for Analyzing Endogenous Tau Fragments in Cerebrospinal Fluid**; Kaushi Ohta[1]; Yusaku Hioki[1]; Rie Yamamoto[1]; Masaki Murase[1]; Koichi Tanaka[1]; *[1]Shimadzu Corporation, Nakagyo-ku, Japan*

WP 084 **HiSorb TD-GC-MS Innovation: Probing Liver Metabolism with Deuterated EVOCs Unveils Potential Novel Enzymatic Pathways and Biomarkers for Disease Diagnosis**; Antonio Murgia[1]; Yusuf Ahmed[1]; Iris Banda[1]; Menisha Manhota[1]; Olga Gandelman[1]; Max Allsworth[1]; Billy Boyle[1]; Daniela Fonseca[1]; Jacob Rudman[1]; Connor Clarke[1]; Alexandra Martin[1]; Giuseppe Ferrandino[1]; *[1]Owlstone Medical Ltd, Cambridge, United Kingdom*

WP 085 **An deep plasma workflow applied to discover biomarker candidates of the response to chemo-immunotherapy in patients with thoracic malignancies**; Stefanie Hiltbrunner[1]; Yuehan Feng[2]; Sandra Schaer[2]; Angelica Rigutto[1]; Polina Shichkova[2]; Christopher Below[2]; Luca Raess[2]; Lukas Reiter[2]; Roland Bruderer[2]; Roger Von Moos[3]; Markus Joerger[3]; Alessandra Curioni-Fontecedro[1, 3, 4]; *[1]University of Fribourg, Faculty of Science and Medicine, Fribourg, Switzerland; [2]Biognosys AG, Schlieren, Switzerland; [3]Swiss Group for Clinical Cancer Research, Bern, Switzerland; [4]Clinic of Oncology, Cantonal Hospital Fribourg, Fribourg, Switzerland*

WP 086 **Linking local and systemic dysregulations in compromised bone healing under diabetic conditions by proteomics analyses**; Johannes R. Schmidt[1]; Vivien Wiltzsch[1]; Klaudia Adamowicz[2]; Lis Arend[3]; Chit Tong Lio[2]; Daniela Dias[4]; Jörg Lehmann[1]; Thomas Lingner[5]; Olga Tsoy[2]; Patrina S.P. Poh[4]; Tanja Laske[2]; Jan Baumbach[2]; Stefan Kalkhof[1, 6]; *[1]Department of Preclinical Development and Validation, Fraunhofer Institute for Cell Therapy and Immunology IZI, Leipzig, Germany; [2]Institute for Computational Systems Biology, University of Hamburg, Hamburg, Germany; [3]Data Science in Systems Biology, Technical University of Munich, Munich, Germany; [4]Julius Wolff Institute, BIH at Charité – Universitätsmedizin Berlin, Berlin, Germany; [5]Genevention GmBH, Göttingen, Germany; [6]Institute for Bioanalysis, Coburg University of Applied Sciences and Arts, Coburg, Germany*

WP 087 **Proteomics Profiling of Mdk Knockout/5xFAD Mice**; Shu Yang[1]; Ya Huang[1]; Zhiping Wu[1]; Yun Jiao[1]; Ping-Chung Chen[1]; Junmin Peng[1]; *[1]St Jude Children's Research Hospital, Memphis, TN*

WP 088 **Exploring the Interplay of Brain Tumors and Neurodegenerative Disorders: A Comprehensive Big Data Analysis**; Sanjeeva Srivastava[1]; Deeptarup Biswas[1]; Sanjyot Vinayak Shenoy[1]; Ankit Halder[1]; Aparna Chauhan[1]; Advait Padhye[1]; Yash Choudhary[1]; *[1]IIT Bombay, Mumbai, India*

WP 089 **Correlation of metabolomics-derived biomarkers for radiation-induced injury with clinical outcome assessments**; Swarnima Pandey[1]; Nageswara Pilli[1]; William T Andrews[1]; Ludovic Muller[1]; Mehari Weldemariam[1]; Maureen A Kane[2]; *[1]University of Maryland, Baltimore, Baltimore, MD; [2]Universityof Maryland, Baltimore, Baltimore, MD*

WP 090 **Proteogenomic analysis of ovarian cancer reveals a signature to predict platinum refractoriness**; Jeff Whiteaker[1]; Shrabanti Chowdhury[2]; Jacob J Kennedy[1]; Richard Ivey[1]; Marcin Cieslik[3]; Pei Wang[2]; Michael Birrer[4]; Amanda Paulovich[1]; *[1]Fred Hutchinson Cancer Research Center, Seattle, WA; [2]Icahn School of Medicine at Mount Sinai, New York, NY; [3]University of Michigan School of Medicine, Ann Arbor, MI; [4]University of Arkansas for Medical Sciences, Little Rock, AR*

WP 091 **The Risk of Using Underpowered Proteomic Studies and the Potential of Using Well-powered Cohorts**; Oliver KO Lindhorst[1]; Dylan Nicholas T Tabang[1, 2]; Arthur Viode[1, 2]; Asher Salmon[1]; Lise Nigrovic[1, 2]; Jonathan R Krieger[3]; Judith A Steen[1, 2]; Hanno Steen[1, 2]; *[1]Boston Children's Hospital, Boston, MA; [2]Harvard Medical School, Boston, MA; [3]Bruker Ltd., Milton, ON*

WP 092 **Unveiling Potential Endogenous Peptide Biomarkers for Hepatocellular Carcinoma in Serum of Patients with Liver Cirrhosis**; Muhammad Salman Sajid[1]; Habtom Ressom[1]; *[1]Georgetown University, Washington, DC*

WP 093 **Exploring Novel Low Abundant Medium Size Serum Protein Biomarkers for Hepatocellular Carcinoma in Patients with Liver Cirrhosis**; Muhammad Salman Sajid[1]; Habtom Ressom[1]; *[1]Georgetown University, Washington, DC*

WP 094 **Dynamic proteomic and phosphoproteomic atlas of neuron maturation with amyloid precursor protein mutation**; Ying Hao[1]; Ziyi Li[1]; Erika Lara Flores[1]; Jasmin Camacho[1]; Benjamin Jin[1]; Lily Cornelius[1]; Sydney Klaisner[1]; Yue A Qi[1]; *[1]National Institutes of Health, Bethesda, MD*

WP 095 **N-Glycosylation of IgA in Ankylosing Spondylitis: Unveiling a Specific Inflammatory Biomarker and Exploring its Potential in Macrophage-Driven Innate Immunity**; Hui-Ling Chiang[1]; Ning-Sheng Lia[1]; Chien-Hsueh Tung[1]; Ming-Chi Lu[1, 2]; Yi-Ling Ye[3]; Chih-Chia Yu[2]; *[1]Division of Immunology, Allergy and Rheumatology, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan; [2]Department of Medical Research, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan; [3]Department of Biotechnology, National Formosa University, Huwei, Taiwan*

WP 096 **Identification of Non-Angiotensin II ACE Products that Enhance Immunity**; Neethu G Issac[1]; Catalina Avendaño[1]; Daniel Röth[1]; Kenneth E. Bernstein[2]; Markus Kalkum[1]; *[1]City of Hope, Beckman Research Institute. Department of Immunology and Theranostics, Duarte, CA; [2]Cedars-Sinai Medical Center, Los Angeles, CA*

WP 097 **Comprehensive workflow for extraction, purification, and accelerated digestion of proteins from Mammalian cells**; Debadeep Bhattacharyya[1]; Patrick McCarthy[2];

Sameer Vasantgadkar[2]; Elisabeth Pundt[2]; Eugenio Daviso[2]; Ulrich Thomann[2]; *[1]Covaris, Lexington, MA; [2]Covaris, LLC, Woburn, MA*

WP 098 **High throughput mass spectrometry measure of metabolites and lipids across human populations**; Mo Jain[1]; Jeramie Watrous[1]; Tao Long[1]; Saumya Tiwari[1]; Tanya Nguyen[1]; Kate Gallagher[1]; *[1]Sapient, San Diego, CA*

WP 099 **Blood metabolome profiling reveals markers for diabetes-associated kidney disease in Asian Indians**; Sneha Rana[1]; Vivek Mishra[2]; Prajval Nakrani[2]; Lakshman Kumar[3]; Manisha Sahay[3]; Rakesh Sahay[3]; Pramod P. Wangikar[1, 2]; *[1]Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai, India; [2]Clarity Bio Systems India Pvt. Ltd., Pune, India; [3]osmania medical college, Hyderabad, India*

WP 100 **Investigation of the effects of overexpression of Human Jumping Translocation Breakpoint (JTB) Protein using in-solution digestion-based Proteomics**; Taniya Modhishika Jayaweera[1]; Madhuri Jayathirtha[1]; Danielle Whitham[1]; Costel C. Darie[1]; *[1]Biochemistry and Proteomics Laboratories, Department of Chemistry and Biomolecular Science,Clarkson University, Potsdam, NY*

WP 101 **Evaluation of Extracellular Vesicle Isolation Methods from CSF for high-throughput HD Biomarkers Identification** ; Chrisovalantis Papadopoulos[1]; Mari Aaltonen[2]; Olga Shatnyeva[3]; Elena Kunold[2]; Thomas Wild[2]; Carleen M Kluger[2]; Doris Staudt[2]; Christoph Schaab[2]; Denise Hartung[3]; Kristin Schneider[4]; Nora Olszok[4]; Farah Aqel[3]; Jim Rosinski[5]; Jian Chen[5]; Thomas F. Vogt[5]; Ramee Lee[5]; *[1]Evotec SE, Hamburg, Germany; [2]Evotec München GmbH, Neuried, Germany; [3]Evotec International GmbH, Göttingen, Germany; [4]Evotec SE, Göttingen, Germany; [5]CHDI Foundation, Princeton, NJ*

WP 102 **Peptidomic analysis of breast milk and serum from donors with Breast Cancer and matched Controls for biomarker discovery**; Pathea S. Bruno[1]; Danielle Whitham[1]; Isabella Pelkey[1]; Brian T. Pentecost[1, 2]; Kathleen F. Arcaro[2]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]University of Massachusetts Amherst, Amherst, MA*

BIOMARKERS: QUANTITATIVE ANALYSIS II
103-128

WP 103 **Mitochondrial quantitative proteomics unveils hypoxia-induced cardiac impairment concomitant increasing of mitochondrial protein**; Pengcheng Fan; *Pharmaron, Germantown, MD*

WP 104 **Improved liquid chromatography-tandem mass spectrometry analysis of isomeric urinary mercapturic acid metabolites of crotonaldehyde, methacrolein, and methyl vinyl ketone**; Menglan Chen[1]; Steven Carmella[1]; Yingchun Zhao[1]; Stephen Hecht[1]; *[1]Masonic Cancer Center, UMN, Minneapolis, MN*

WP 105 **Short and Long-term Stability of tobacco specific Nitrosamines (TSNAs) in human Urine**; Baoyun Xia[1]; Vivian Lee[1]; Alexandria-Helen Rollins[1]; Katie Harbin[1]; John Lee[1]; Justin Lamar Brown[1]; Christina Brosius[1]; Tonya Guillot[1]; Chelsea Walker[1]; Lanqing Wang[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

WP 106 **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[1]; Tian-Sheng Lu[1]; Shuyu Hou[1]; *[1]Medpace, Cincinnati, OH*

WP 107 **Enhancing BBB Integrity Biomarker Quantitation in Neurovascular Disorder Research through Microflow Solutions**; Dhavalkumar Patel[1]; Ehsan Nozohouri[1]; Ebru Selen[2]; Rahul Baghla[2]; Ulrich Bickel[1]; *[1]Texas Tech University Health Sciences Center, Amarillo, TX; [2]SCIEX, Redwood City, CA*

WP 108 **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[1]; Lori Lollis Fralick[1]; Kelly Frances Ethun[1]; *[1]Biomarker Core, Emory National Primate Research Center, Emory University, Atlanta, GA*

WP 109 **High-resolution mass spectrometry peptide quantitation for biomarker verification using data-independent acquisition**; Remco Van Soest[1]; Patrick Pribil[2]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Concord, ON*

WP 110 **Achieving Improved Precision and Low Carryover in Parallel Reaction Monitoring Mass Spectrometry through Optimized Chromatographic Strategies with uPAC Neo Column**; Yuan Lin[1]; Jeff Op De Beeck[2]; Paul Jacobs[2]; Shanhua Lin[1]; *[1]Thermo Fisher Scientific, Sunnyvale, CA; [2]Thermo Fisher Scientific, Ghent, Belgium*

WP 111 **Maximizing detector utilization – Dual-HPLC-MS for the rapid quantification of metabolites in human blood**; Christian Faist[1]; Thorsten Eierhoff[2]; Heiko Hayen[1]; *[1]University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; [2]University Hospital Muenster, Department of Vascular and Endovascular Surgery, Münster, Germany*

WP 112 **Stability of Urinary Cotinine and Trans-3’-hydroxycotinine Measurements across 2012-2023**; Patrick Bendik[1]; June Feng[1]; Lanqing Wang[1]; *[1]CDC, Atlanta, GA*

WP 113 **A sensitive HPLC-MS/MS Method for the Determination of Propylene Glycol in Human Plasma Using Surrogate Standard Approach**; Yizhong Zhang[1]; Wenyan Tang[2]; Brian Hee, [3]; Qiang Wang[1]; Changming Yang[2]; Wenzhong Liang[2]; Sakambari Tripathy[1]; Katty Wan, [3]; *[1]Pfizer Inc., Groton, CT; [2]WuXi AppTec (Shanghai) Co., Ltd, Shanghai, China; [3]Pfizer Inc., San Diego, CA*

WP 114 **Advantages of complementary library construction for the identification and quantification of biomarkers for kidney-related diseases from human plasma**; Jake T Kline[1]; Philip M. Remes[2]; Cristina Jacob[2]; Lilian R Heil[2]; Charles Maxey[2]; Stephanie Samra[2]; Scott M Peterman[2]; Claudia Martins[2]; Lorenzo Gallon[3]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]Thermo Fisher Scientific, San Jose, CA; [3]University of Illinois Chicago, Chicago, IL*

WP 115 **Analysis of Hemorphin Levels in Sickle Cell Disease using PRM-PASEF and Its Association to Pain**; Yanqi Tan[1]; Eduardo De La Toba[1]; Yavnika Kashyap[2]; Robert Molokie[2, 3]; Jim Wang[2]; Jonathan Sweedler[1]; *[1]Department of Chemistry, University of Illinois Urbana-Champaign, Urbana, Illinois; [2]Department of Pharmaceutical Sciences, University of Illinois Chicago, Chicago, Illinois; [3]Department of Medicine, University of Illinois Chicago, Chicago, Illinois*

WP 116 **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[1]; Eric Thomas[1]; *[1]Labcorp Bioanalytical Services LLC, Indianapolis, IN*

WP 117 **De Novo Assay Development to Quantify Low Abundant Protein Biomarkers by Immunocapture-LC-MS/MS for Cancer Immunotherapy Development**; Naiyu Zheng[1]; Kristin Taylor[1]; Jennifer Postelnek[1]; Sagar Kawle[1]; Huidong Gu[1]; Tracy Tang[1]; Ming Lei[1]; Sonia Dolfi[1]; Graham Yearwood[1]; Jianing Zeng[1]; *[1]Bristol Myers Squibb, Princeton, NJ*

WP 118 **Plasma Biomarkers Discovery of Multiple System Atrophy Disease Based on Proteomic Landscape**; Longqin Sun[1]; Jingli Li[1]; Songfeng Wu[1]; Ruibing Li[2]; Yan Zhao[1]; *[1]Beijing Qinglian Biotech Co., Ltd,, Beijing, China; [2]the First Medical Centre, Chinese PLA General Hospital, Beijing, China*

WP 119 **Magnetic Beads Based Solid Phase Extraction—Innovative Technology for Automated Sample Preparation**; Qunjie Wang; *Suzhou Agile Bio Electronic Technology Co. LTD., Suzhou, China*

WP 120 **Developement of a blood-based multiplex sensitive LC-MS method for neurodegenerative diseases patient stratification : towards an innovative diagnostic tool**; Florine Leipp[1, 2]; Jérôme Vialaret[2]; Aurore Jaffuel[3]; Ann-Christin Niehoff[4]; Sylvain Lehmann[2]; Christophe Hirtz[2]; *[1]Shimadzu France, Noisiel, France; [2]LBPC-PPC, Montpellier*

University, IRMB CHU Montpellier, INM INSERM, Montpellier, France; [3]Shimadzu Corporation, Nakagyo-ku, Japan; [4]Shimadzu Europa GmbH, Duisburg, Germany

WP 121 **Development and Validation of a Liquid Chromatography Tandem Mass Spectrometry Assay for the Quantification of Dapivirine in Human Hair**; Hideaki Okochi[1]; Alexander Louie[1]; Erica Beckerdite[1]; Karen Kuncze[1]; Edward W. Livant[2]; Leslie Z. Benet[1]; Thesla Palanee-Phillips[3, 4]; Nyaradzo M. Mgodi[5]; Monica Gandhi[1]; *[1]University of California-San Francisco, San Francisco, CA; [2]Magee Womens Research Institute, Pittsburgh, PA; [3]University of the Witwatersrand, Johannesburg, South Africa; [4]University of Washingon, Seattle, WA; [5]University of Zimbabwe, Harare, Zimbabwe*

WP 122 **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 123 **A simple derivatization LC/MS/MS method for the quantitation of plasma short-chain fatty acids**; Anna M. Caldwell[1]; Nur N. Z. Kamarunzaman[1]; Ana Rodriguez-Mateos[1]; John M. Halket[1]; *[1]King's College London, London, United Kingdom*

WP 124 **Quantification of Frataxin Proteoforms in Blood of Carriers as Biomarkers of Friedreich's Ataxia Using a Triple Quadrupole Mass Spectrometer**; Teerapat Rojsajjakul[1]; David R. Lynch[1]; Clementina Mesaros[1]; Ian Alexander Blair[1]; *[1]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*

WP 125 **Develop and Validated an Ultra-sensitive LC-MS/MS Method to Simultaneously Quantify Aldosterone and Other 4 Steroids in Human Plasma**; Yuhuan Ji[1]; Chenggang Li[1]; Changjian Zhao[1]; Min Meng[1]; Laixin Wang[1]; *[1]Resolian China, Chongqing, China*

WP 126 **Comprehensive profiling of data acquisition strategies to optimize clinically-feasible approaches for monitoring predictive phosphorylation markers**; Amy E Campbell[1]; Pedro Moreno-Cardoso[1]; Luis Nobre[1]; David N Perkins[1]; Josie A Christopher[1]; Janet Kelsall[1]; Weronika E Borek[1]; Andrew Williamson[1]; Arran D Dokal[1]; *[1]Kinomica Ltd, Macclesfield, United Kingdom*

WP 127 **Quantitative Analysis of Amino Acids and Acylcarnitines from Isotope-Impregnated Dried Blood Spots Using Mass Spectrometry**; Wenqian Li[1]; Donald H. Chace[2]; Timothy J. Garrett[1]; *[1]University of Florida, GAINESVILLE, FL; [2]Capitainer miQro lab, Warwick, Rhode Island*

WP 128 **Long-term reproducibility of trace-level quantification of seven PAH biomarkers in urine by on-line SPE-HPLC-MS/MS**; Yuesong Wang[1]; Erin N. Pittman[1]; Debra A. Trinidad[1]; Kyle Smith[1]; Antonia M. Calafat[1]; Julianne Cook Botelho[1]; *[1]CDC, Atlanta, GA*

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WP 130 **Deciphering Proteome-wise Regulatory Landscape of Ferroptosis in Non-Small Cell Lung Cancer**; Xuan Mo[1]; Carlo P. Ramil[1]; Kerrie Simon[1]; Benjamin Ruprecht[1]; An Chi[1]; *[1]Chemical Biology, Merck & Co., Inc., Cambridge, MA*

WP 131 **Acalabrutinib and Potential drug-induced organ toxicity (DIOT): Bioactivation characterized by Mass Spectrometry**; Aishah M Alsibaee[1]; Haya I Aljohar[1]; Mohamed W. Attwa[1]; Ali S Abdelhameed[1]; Adnan A Kadi[1]; *[1]College of Pharmacy, King Saud University, Riyadh, SA, Riyadh, Saudi Arabia*

WP 132 **Assessing Long-Term Stored Tissues for Multi-Omics Data Quality and Proteogenomics Suitability**; Kyujin Song[1]; Jae-Won Oh[1]; Eunok Paek[2, 3, 4]; Joon-Yong An[5, 6, 7]; Se Jin Jang[8]; Min-Sik Kim[9, 10, 11]; Kwang Pyo Kim[1, 12]; *[1]Kyung-Hee University, Yong-in, South Korea; [2]Department of Computer Science, Hanyang University, Seoul, South Korea; [3]Institute for Artificial Intelligence Research, Hanyang University, Seoul, South Korea; [4]Department of Artificial Intelligence, Hanyang University, Seoul, South Korea; [5]Department of Integrated Biomedical and Life Science, Korea University, Seoul, South Korea; [6]BK21FOUR R&E Center for Learning Health Systems, Korea University, Seoul, South Korea; [7]School of Biosystem and Biomedical Science, College of Health Science, Korea University, Seoul, South Korea; [8]University of Ulsan College of Medicine, Asan Medical Center,, Seoul, South Korea; [9]Department of New Biology, Daegu Gyeongbuk Institute of Science and Technology, Daegu, South Korea; [10]New Biology Research Center, DGIST, Daegu, South Korea; [11]Center for Cell Fate Reprogramming and Control, DGIST, Daegu, South Korea; [12]Kyung Hee Medical Science Research Institute, Seoul, South Korea*

WP 133 **Coupled Proteomic-Bioinformatic Approach to Investigate New Potential Therapeutic Targets for Soft Tissue Sarcoma**; Veronica De Giorgis[1]; Vittoria Federica Borrini[2]; Marcello Manfredi[1]; Virginia Vita Vanella[1]; Elettra Barberis[2]; Maria Rescigno[3]; Luca Tiraboschi[3]; *[1]Department of Translational Medicine, University of Piemonte Orientale, Novara, Italy; [2]Department of science technological innovation, University of Piemonte Orientale, Alessandria, Italy; [3]Clinical institute Humanitas IRCCS, Milan, Italy*

WP 134 **Mass spectrometry identifies novel interactors and palmitoylation targets of zDHHC23 in neuroblastoma**; Sally O Oswald[1, 2]; Leonard A Daly[2, 3]; Barry Pizer[3, 4]; Ian A Prior[3]; Violaine See[5]; Claire E Eyers[2, 3]; *[1]University of Liverpool, Liverpool, United Kingdom; [2]Centre for Proteome Research, Liverpool, United Kingdom; [3]University of Liverpool, Liverpool, United Kingdom; [4]Alder Hey Children's Hospital, Liverpool, United Kingdom; [5]Université de Lyon, Lyon, France*

WP 135 **CETSA MS profile of five breast cancer cell lines correlates with their biological response to clinically used breast cancer medicines**; Tuomas A Tolvanen[1]; Tomas Friman[1]; Merve Kacal[1]; Ying Sun[1]; Laurence Arnold[1]; Daniel Martinez Molina[1]; *[1]Pelago Bioscience AB, Solna, Sweden*

WP 136 **Ultra-Deep Proteome of Osteosarcoma Unravels Novel Biomarkers for Drug Targeting**; Joris Maximilian Frenz[1, 2, 3]; Lianghao Mao[2, 3]; Noelle Jung[1, 3]; Dibyendu Seal[1, 3]; Yongjie Wang[1, 3]; Robert Autry[1, 3]; Stefan M. Pfister[1, 3]; Andreas Von Deimling[2]; Andreas E. Kulozik[1, 2, 3]; Ashok Kumar Jayavelu[1, 3]; *[1]German Cancer Research Center (DKFZ), Heidelberg, Germany; [2]Heidelberg University Hospital (UKHD), Heidelberg, Germany; [3]Hopp Children's Cancer Center (KiTZ), Heidelberg, Germany*

WP 137 **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 138 **Identifying possible new CAR-T cell immunotherapy targets induced by drug treatment with surface proteomics**; Ruzena Filandrova[1]; Pauline Douglas[1]; Sorana Morrissy[1]; Jennifer Chan[1]; David C Schriemer[1]; *[1]University of Calgary, Calgary, AB*

WP 139 **Proteomic Analysis of Red Blood Cells Reveals Putative Biomarkers of Prostate Cancer**; Tong Zhang[1]; Zhangyang Xu[2]; Rachel Lawrence[3]; Priscila Lalli[2]; Yongjie Lu[3]; Tujin Shi[2]; *[1]Pacific Northwest National Lab, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Queen Mary University of London, London, United Kingdom*

WP 140 **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[1]; Getulio Pereira De Oliveira Junior[1]; Jacqueline Wood[1]; Alexander R. Ivanov[1]; *[1]Northeastern University, Boston, MA*

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WP 143 **Identification and quantification of candidate protein biomarkers in human plasma for early diagnosis of breast cancer**; Margret Thorsteinsdottir[1, 2, 3]; Kristrun Yr Holm[1, 2]; Magnus Gauti Ulfarsson[1, 3]; Valdis Gunnarsdottir Thormar[2, 4]; Finnur Freyr Eiriksson[1, 3]; Yassene Mohammed[5, 6]; Christoph H. Borchers[6, 7, 8, 9]; Sigridur Klara Bodvardsdottir[2, 4]; *[1]Faculty of Pharmaceutical Sciences, University of Iceland, Reykjavik, Iceland; [2]BioMedical Center, University of Iceland, Reykjavik, Iceland; [3]ArcticMass, Reykjavik, Iceland; [4]Faculty of Medicine, University of Iceland, Reykjavik, Iceland; [5]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [6]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, McGill University, Montreal, Quebec; [7]Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; [8]Division of Experimental Medicine, McGill University, Montreal, QC; [9]Department of Pathology, McGill University, Montreal, QC*

WP 144 **Developing a multiplexed proteoform reaction monitoring (PfRM) assay for the quantification of intact RAS proteins from cancer cell lines**; Alyssa A Williams[1]; Jake T Kline[1]; Robert A D'Ippolito[2]; Grace M Scheidemantle[2]; Peter H Frank[2]; Dominic Esposito[2]; Caroline J DeHart[2]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]Frederick National Laboratory for Cancer Research, Frederick, MD*

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WP 146 **Molecularly Aware Robotic Surgery with Laser Desorption – Rapid Evaporative Ionisation Mass Spectrometry for Autonomous Surgical Interventions**; Jinshi Zhao[1]; Daniel Simon[1, 2]; Mark Runciman[1]; Haozheng Xu[1]; Amelia Fraser-Dale[1]; Eftychios Manoli[1]; Stamatia Giannarou[1]; George Mylonas[1]; Zoltan Takats[1, 2]; Burak Temelkuran[1, 2]; *[1]Imperial College London, London, United Kingdom; [2]Rosalind Franklin Institute, Harwell, United Kingdom*

WP 147 **Assessment of global metabolic changes in antibiotic treated mice and the impact on the pancreatic cancer tumor microenvironment**; Dominik Awad[1]; Li Zhang[1]; Peter Sajjakulnukit[1]; Harrison Wong[1]; Anthony Andren[1]; Damien Sutton[1]; Noah Nelson[1]; Carlos Espinoza[1]; Donnele Daley[1]; Costas A Lyssiotis[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 148 **Extracellular vesicles' lipidome differs between types of cancers as well as between primary and metastatic cancers**; Erika Dorado[1]; James S McKenzie[1]; Stefania Maneta-Stavrakaki[1]; R Charles Coombes[1]; Zoltan Takats[1]; *[1]Imperial College London, London, United Kingdom*

WP 149 **Studying crosstalk between tumor and microenvironmental cells driving drug response in Acute Myeloid Leukemia using cell-type specific proteomics**; Marija Veličković[1]; Hsin-Yun Lin[2]; Belinda B Garana[1]; Marina A Gritsenko[1]; Reta Birhanu Kitata[1]; Thomas L. Fillmore[1]; Karl K. Weitz[1]; Jeffrey J. Tyner[2]; Sara J.C. Gosline[1]; Anupriya Agarwal[2]; Paul D. Piehowski[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Oregon Health and Science University, Portland, OR*

WP 150 **Protein biomarker discovery across stages of pancreatic neoplasms using mass-spectrometry based proteomics of pancreatic cyst fluid**; Gina Chang[1]; Whitney Smith-Kinnaman[1]; Amber L Mosley[1]; *[1]Indiana University School of Medicine, Indianapolis, IN*

WP 151 **Thermal Proteome Profiling to discover novel protein targets of PARP inhibitors**; Li Wang[1]; Jidong Wang[2]; Xiangyi Kong[2]; MD Kamrul Hasan Khan[2]; Xinyan Wu[2]; *[1]Mayo clinic, Rochester, MN; [2]Mayo Clinic, Rochester, MN*

WP 152 **Mass spectrometry-based bulk and single-cell proteomic profiling of CB-5083 resistant colon cancer cells**; Marion Pang[1]; Ting-Yu Wang[1]; Feng Wang[1]; Shan Li[1]; Chai Foong Lai[1]; Baiyi Quan[1]; Yanping Qiu[1]; Tsui-Fen Chou[1]; *[1]California Institute of Technology, Pasadena, CA*

WP 153 **Comparison of Mass Spectrometry-Based Proteomics Data from Primary Human and Patient-Derived Xenograft Mouse Tumors**; Fernando Garcia-Marques[1, 2]; Abel Bermudez[1, 2]; Dalin Zhang[3]; Hongjuan Zhao[3]; James D. Brooks[3]; Sharon J Pitteri[1, 4]; *[1]Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; [2]Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; [3]Department of Urology, Stanford University School of Medicine, Stanford, CA 94305, Palo Alto, CA; [4]Department of Radiology, Stanford University School of Medicine, Palo Alto, CA, United States, Palo Alto, CA*

WP 154 **Recurrence In Hepatocarcinoma Investigated With Picosecond Infrared Laser Mass Spectrometry: Towards A Rapid Screening Tool For Successful Transplant**; Francis O Talbot[1]; Lan Anna Ye[1]; Michael Woolman[1]; Arash Zarrine-Afsar[2]; Elisa Pasini[1]; Xun Zhao[1]; Jeffery To[1]; Mamatha Bhat[1]; *[1]University Health Network, Toronto, ON; [2]Princess Margaret Cancer Centre, University Health Network, Toronto, ON*

WP 155 **Deciphering Medulloblastoma Heterogeneity in the Indian Subpopulation: An FFPE-Based Proteomic Study**; Medha Gayathri J Pai[1]; Avinash Singh[1]; Shilpa Rao[2]; Anita Mahadevan[2]; Sanjeeva Srivastava[1]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]National Institute of Mental Health and Neurological Sciences, Bengaluru, India*

WP 156 **Discovery and validation of secretory markers-derived from sphingolipid metabolism in Oral Squamous Cell Carcinoma patients through discovery and targeted proteomics**; Avinash Singh[1]; Suraj T[1]; Abhinav Verma[2]; Richa Vaish[3]; Sudhir Nair[4]; Sanjeeva Srivastava[1]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Indian Institute of Science Education and Research, Berhampur, India; [3]Tata Memorial Hospital, Mumbai, India; [4]Advance Centre for Treatment Research & Education in Cancer, Mumbai, India*

WP 157 **Multi-Omics Approach based Drug Discovery: Unleashing targets pertaining to Meningioma aggressiveness and evaluating the drug efficacy**; Ankit Halder[1]; Deeptarup Biswas[1]; Archisman Maitra[1]; Sanjeeva Srivastava[1]; *[1]Indian Institute of Technology Bombay, Mumbai, India*

WP 158 **Mass spectrometry-based characterization of oxidative damage for different dose rate regimes as a new platform for investigating the FLASH effect**; Sayan Gupta[1]; Jamie Inman[1]; Jared De Chant[1]; Lieselotte Obst-Huebl[1]; Kei Nakamura[1]; Shawn Costello[2]; Darren Kahan[3]; Susan Marqusee[3]; Jian-Hua Mao[1]; Louis Kunz[4]; Marie-Catherine Vozenin[5]; Antoine Snijders[1]; Corie Y Ralston[1]; *[1]Lawrence Berkeley National Laboratory, Berkeley, CA; [2]Stanford University, Stanford, CA; [3]University of California, Berkeley, Berkeley, CA; [4]Hôpitaux Universitaires de Genève, Geneva, Switzerland; [5]Hôpitaux Universitaires, Geneva, Switzerland*

WP 159 **Characterization of the Cell-Membrane Proteome as the Interface Between Cancer Cells and the Tumor Microenvironment**; Iulia M. Lazar[1]; Yunqian Zhang[1];

Pratistha Sarkar[1]; Joshua RS Haueis[1]; Shreya Ahuja[1]; Arba Karcini[1]; [1]*Virginia Tech, Blacksburg, Virginia*

WP 160 **Proteomic Insights of FAK Dependency in Breast Cancer**; Lai Chai Foong[1]; Hope Hua[1]; Wenxuan Huang[1]; Chia Yen Liew[2]; Diana Huynh[1]; Ting-Yu Wang[2]; Baiyi Quan[2]; Yanping Qiu[2]; Timothy Marlowe[3]; Gordon Stott[4]; Andrew Flint[4]; Barbara Mroczkowski[5]; Tsui-Fen Chou[1, 2]; [1]*Division of Biology and Biological Engineering, California Institute of Technology, Pasadena, CA;* [2]*Proteome Exploration Laboratory, Beckman Institute, California Institute of Technology, Pasadena, CA;* [3]*The University of Arizona Cancer Center, Phoenix, AZ;* [4]*Leidos Biomedical Research, Inc., Frederick National Laboratory for Cancer Research, National Cancer Institute, Bethesda, MD;* [5]*Division of Cancer Diagnosis and Treatment and Center for Cancer Research, NCI, NIH, Bethesda, MD*

WP 161 **Comprehensive proteogenomic investigation of high-grade gliomas towards identifying markers of therapeutic potential and drug repurposing for drug candidates**; Ayushi Verma[1]; Prashant Kumar[2]; Sanjeeva Srivastava[3]; [1]*Indian Institute of Technology Bombay, Mumbai, India;* [2]*Karkinos Lab, Mumbai, India;* [3]*Indian Institute of Technology Bombay, Mumbai, India*

WP 162 **Extracellular Vesicle Proteomics of Primary Human Monocyte-Derived Myeloid Cells**; Carlo Ramil[1]; Handan Xiang[1]; Lisia Cabral[1]; Zhizhang Yin[1]; An Chi[1]; [1]*Merck & Co., Inc., Cambridge, MA*

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WP 165 **Mechanistic insights into the antitumoral potential of a new silver/selenium based nanosystem revealed by mass spectrometry**; Jose L Luque-Garcia[1]; Pilar Buenadia-Nacarino[1]; Roberto Alvarez-Fernandez Garcia[1]; Blanca Gonzalez[1]; [1]*Complutense University of Madrid, Madrid, Spain*

WP 166 **A mass spectrometry-based multi-omic approach for the evaluation of rhodium nanoparticles as novel photosensitizers in photodynamic therapy for cancer**; Gabriel A. Peñalver[1]; Andres Machuca[1]; Alejandro Garcia-Garcia[1]; Estefania Garcia-Calvo[1]; Jose L Luque-Garcia[1]; [1]*Complutense University of Madrid, Madrid, Spain*

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WP 168 **The Clinical Application of Monitoring of Voriconazole and Its Metabolites in Allogeneic Hematopoietic Stem Cell Transplantation Patients**; Wang hong Chun[1]; Wang Lei[2]; [1]*Beijing Lu Daopei Hospital, 22 Tongji Nan Road, Tongzhou District, Beijing, Beijing, China;* [2]*Hebei Yanda Lu Daopei Hospital, Langfang, China*

WP 169 **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[1]; Justin Steimling[2]; [1]*Restek Inc., Bellefonte, PA;* [2]*Restek Corporation, Bellefonte, PA*

WP 170 **Untargeted Paper Spray Mass Spectrometry (PS-MS): Rapid Diagnosis of Albuminuria Enabling Early Detection and Progression Monitoring of Chronic Kidney Disease**; Igor Pereira[1]; Jindar N.S. Sboto[1]; Jason L Robinson[2]; Christopher G. Gill[1, 3, 4, 5, 6]; [1]*Appl. Env. Res. Labs. (AERL), Nanaimo, BC;* [2]*Health PEI, Charlottetown, PEI;* [3]*Vancouver Island University, Nanaimo, BC;* [4]*University of Victoria, Victoria, BC;* [5]*Simon Fraser University, Burnaby, BC;* [6]*University of Washington, Seattle, WA*

WP 171 **Biomarkers of parenteral nutrition in newborns and their utility in newborn screening**; Konstantinos Petritis[1]; C. Austin Pickens[1]; Rachel C. Lee[1]; Carla D. Cuthbert[1]; [1]*Centers for Disease Control and Prevention, Atlanta, GA*

WP 172 **Amplification of collision cross-section differences in metal ions by supramolecular complexation with calixarenes in a Bruker timsTOF instrument**; Liu Yang[1]; Jun J Hu[1]; Fuxing Xu[1]; [1]*Ningbo University, Ningbo, China*

WP 173 **MONITORING OVULATION BY MEASUREMENT OF PREGNANEDIOL-3-GLUCURONIDE IN SPOT URINE SAMPLES VIA UHPLC-MS/MS**; Laura Leoni[1]; Federico Ponzetto[2]; Federica Rosmini[3]; Mirko Parasiliti Caprino[2]; Fabio Settanni[4]; Antonello Nonnato[4]; Ezio Ghigo[2]; Paolo Moghetti[3]; Giulio Mengozzi[1, 4]; [1]*Clinical Biochemistry Laboratory, Department of Medical Sciences, University of Turin, Turin, Italy;* [2]*Endocrinology, Diabetology and Metabolism, Department of Medical Sciences, University of Turin, Turin, Italy;* [3]*Endocrinology, Diabetes and Metabolism, Department of Medicine, University of Verona, Verona, Italy;* [4]*Clinical Biochemistry Laboratory, City of Health and Science University Hospital, Turin, Turin, Italy*

WP 174 **Improving Lung Cancer Diagnosis: Exploring the Potential of the MasSpec Pen in non-small cell lung cancer Detection and Subtyping**; Yasmin Shanneik[1]; Bryan Burt[2]; Maheshwari Ramineni[1]; Livia S. Eberlin[1]; [1]*Baylor College of Medicine, Houston, TX;* [2]*University of California, Los Angeles, Los Angeles, CA*

WP 175 **Collection of trace blood using dedicated device and simultaneous analysis of immunosuppressive drugs in whole blood samples**; Takahiro Goda[1]; Yuki Suzuki[2]; Junichi Masuda[2]; Natsuka Kimura[3]; Kenichi Aizawa[3]; [1]*SHIMADZU Corporation, Kawasaki, Japan;* [2]*SHIMADZU Corporation, Kawasaki, Japan;* [3]*Jichi Medical University, Shimotsuke, Japan*

WP 176 **Validation of a new fully automated assay of Thiamine-PyroPhosphate and Pyridixal-5-Phosphate in whole blood using LC-MS/MS**; Joep Vuurpijl[1]; Dennis Van Den Heuvel[2]; Chantal Wilbers[1]; Rein Hoedemakers[1]; Tom Stokhof De Jong[2]; [1]*Jeroen Bosch Ziekenhuis, 's-Hertogenbosch, Netherlands;* [2]*Shimadzu Benelux, 's-Hertogenbosch, Netherlands*

WP 177 **Paper Spray Mass Spectrometry Utilizing On-Paper Enzyme Hydrolysis of Glucuronide Metabolites for Rapid Drug Quantitation in Urine**; Taelor M. Zarkovic[1, 2]; Christopher G. Gill[1, 2, 3, 4, 5]; [1]*Appl. Env. Res. Labs. (AERL), Nanaimo, BC;* [2]*University of Victoria, Victoria, BC;* [3]*Vancouver Island University, Nanaimo, BC;* [4]*Simon Fraser University, Burnaby, BC;* [5]*University of Washington, seattle, WA*

WP 178 **Quantitative GC-MS Analysis of Feces Short-Chain Fatty Acids: Exploring Intestinal Microbiota-Metabolic Disorders Link in Polycystic Ovary Syndrome**; Evgenii Kukaev[1, 2]; Alisa Tokareva[1]; Ekaterina Kirillova[1]; Galina Chernukha[1]; Natalia Starodubtseva[1, 3]; Vladimir Frankevich[1]; [1]*National Medical Research Center for Obstetrics Gynecology and Perinatology, Moscow, Russia;* [2]*Talrose Institute for Energy Problems of Chemical Physics, Moscow, Russia;* [3]*Moscow institute of physics and technology, Moscow, Russia*

WP 179 **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[1]; DARYL HEE[1]; [1]*Changi General Hospital, Singapore, Singapore*

WP 180 **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[1]; Larissa Campos Motta[1]; Gabriely Silveira Folli[1]; Kelliany da Penha Barcelos Carvalho[2]; Ricardo Alves Bernardo[3]; Almir Custódio Batista Junior[4]; Andréa Rodrigues Chaves[4]; José Brango-Vanegas[5, 6]; Rosiane Andrade Da Costa[5]; Octávio Luiz Franco[5, 6]; Frederico Garcia Pinto[7]; Denise Coutinho Endringer[8]; Valério Garrone Barauna[9]; Paulo Roberto Filgueiras[10]; José Geraldo Mill[9]; Wanderson Romão[1, 11];

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WP 181 **Exploratory Analysis MALDI-TOF MS for Detection of Potential Biomarkers of Acute Kidney Injury in Biofluids from Patients Undergoing Liver Transplantation**; Larissa Campos Motta[1]; Camila Medeiros De Almeida[1]; Gabriely Silveira Folli[1]; José Brango-Vanegas[2]; Rosiane Andrade Da Costa[3]; Octavio Luiz Franco[3, 4]; Paulo Roberto Filgueiras[5]; Paula Frizera Vassalo[6]; Vandack Alencar Nobre Júnior[6]; Valério Garrone Barauna[7]; Wanderson Romao[1, 8]; *[1]Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espirito Santo, Vitória, Brazil; [2]Catholic University of Brasilia, Brasilia, Brazil; [3]Catholic University of Brasilia, Brasilia, Brazil; [4]Dom Bosco Catholic University, Campo Grande, Brazil; [5]Department of Chemistry, Federal University of Espirito Santo, Vitória, Brazil; [6]Federal University of Minas Gerais, Hospital das Clínicas of UFMG., Belo Horizonte, Brazil; [7]Department of Physiological Sciences, Federal University of Espírito Santo, Vitória, Brazil; [8]Federal Institute of Espírito Santo, Brazil, Vila Velha, Brazil*

WP 182 **Inflammatory signature associated with continuous subcutaneous insulin infusion sites (CSII) in Type1 Diabetes: A Proteomic biomarker study from CSII Cannula**; Katarzyna Dabrowska[1]; John Blanchard[2]; Maya Willey[2]; Krystine Garcia-Mansfield[2]; Ritin Sharma[2]; Bithika Thompson[3]; Patrick Pirrotte[2]; Sampath Rangasamy[2]; *[1]City of Hope, Duarte, CA; [2]Translational Genomics Research Institute, Phoenix, AZ; [3]Mayo Clinic, Scottsdale, AZ*

WP 183 **Long-term stability and reproducibility of a nanoparticle-based platform for clinical proteomics of human biofluids**; Carleen M Kluger[1]; Frank Rolfs[1]; Till Kindel[1]; Oliver Kardell[1]; Christian Schiffmann[2]; Barbara Kracher[1]; Andreas Tebbe[1]; *[1]Evotec München GmbH, Neuried, Germany; [2]Evotec International GmbH, Göttingen, Germany*

WP 184 **Paper-Based Immunoassay for Multiplexed Detection of Colorectal Cancer Biomarkers Through Direct Paper Spray Mass Spectrometry**; Girish Muralikrishnan[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio*

WP 185 **Comprehensive Sample Preparation Workflow for Deparaffinizaton, Extraction, Purification, and Accelerated Digestion of Proteins from Formalin-Fixed Paraffin-Embedded Tissue**; Debadeep Bhattacharyya[1]; Patrick McCarthy[2]; Sameer Vasantgadkar[2]; Elisabeth Pundt[2]; Eugenio Daviso[2]; Ulrich Thomann[2]; *[1]Covaris, Lexington, MA; [2]Covaris, LLC, Woburn, MA*

WP 186 **Developing Global Access to Mass Spectrometry through Research Capacity Building Programs**; Waheed Adeola Adedeji[1]; Taona Emmah Mudhuli[2]; Faithful Makita Chingombe[3]; Mario Golding[4]; Jill Hochreiter[5]; Raymond Cha[5]; Qing Ma[5]; Robin Difrancesco[5]; Troy D Wood[5]; Gene D. Morse[5]; *[1]University of Ibadan, Ibadan, Nigeria; [2]Midlands State University, Gweru, Zimbabwe; [3]University of Zimbabwe, Harare, Zimbabwe; [4]University of the West Indies, Kingston, Jamaica; [5]University at Buffalo, Buffalo, NY*

WP 187 **Machine learning assisted MALDI mass spectrometry for rapid antimicrobial resistance prediction in clinicals**; Hang Li[1]; Weibo Gao[1]; Jinming Zhang[1]; Shuang Li[1]; Shuailong Zhang[1]; *[1]Beijing Institute of Technology, Beijing, China*

WP 188 **Novel Cleanup and Derivatization Method for High-Throughput Dried Blood Spot Measurement of Hormones**; Julian Reed; *Molecular Testing Labs, Vancouver, WA*

WP 189 **Quantifying long-term stress levels by analyzing cortisol in hair in 8 seconds**; Sarah Demers[1]; Mélanie Merceur[2]; Mégane Moreau[1]; Serge Auger[1]; Jonathan Rochon[1]; Pierre Picard[1]; Jean Lacoursière[1]; *[1]Phytronix Technologies, Quebec City, QC; [2]Bertin Technologies, Montigny-Le-Bretonneux, France*

WP 190 **Near Real-Time Monitoring of Blood Biomarkers with “Rapid Proteomics”**; Steven Yannone[1]; Simion Kreimer[2, 3]; *[1]CinderBio, Berkeley, CA; [2]Cedars-Sinai, Los Angeles, CA; [3]milliThomson, Los Angeles, CA*

WP 191 **Exploring Different HPLC Column Chemistries for Optimal Separation of 13 Bile Acids by LC-MS/MS**; Haley Berkland[1]; Katharina Schramm[2]; Tatiana Yuzyuk[2]; Paul Connolly[1]; Justin Steimling[1]; Jared Burkhart[1]; *[1]Restek Corporation, Bellefonte, PA; [2]ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT*

WP 192 **Signal-to-noise is not a useful performance metric in quantitative analysis**; Brian A Rappold[1]; Randall K Julian[2]; *[1]LabCorp, Raleigh, NC; [2]Indigo BioAutomation, Carmel, Indiana*

WP 193 **Application of Deuterium Labeling Mass Spectrometry for a Rapid Antimicrobial Resistance Assay of ESKAPEE Pathogens**; Josiah Rensner[1]; Paul Lueth[1]; Bryan Bellaire[1]; Orhan Sahin[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

WP 194 **Quantitation of endogenous steroids in serum using plasma separation cards and triple quadruple mass spectrometry**; Vikki Johnson[1]; Nicholas Chestara[2]; Yoshiyuki Okamura[3]; *[1]Shimadzu Scientific Instruments, Carlsbad, CA; [2]DPX Technologies, La Jolla, CA; [3]Shimadzu Scientific Instruments, Columbia, MD*

WP 195 **Dual nESI/APCI source for Analysis of Complex Mixtures**; RILEY FERGUSON[1]; Dmytro S Kulyk[1]; Abraham Kwame Badu Tawiah[1]; *[1]Ohio State University, Columbus, OH*

WP 196 **Elevating Excellence: Pioneering a Holistic Strategy to Minimize Carryover and Boost Precision in Plasma Proteomic Discoveries**; Dave Quilici[1]; Brett Phinney[2]; Michael Krawitzky[3, 4]; Pierre-Olivier Schmit[5]; *[1]University of Nevada Reno, Reno, NV; [2]University of California Davis, Davis, CA; [3]Bruker Daltonics, San Jose, CA; [4]Bruker Switzerland AG, Faellanden, Switzerland; [5]Bruker France SAS, Wissembourg, France*

WP 197 **Development And Validation Of New Method To Measure Plasma Aldosterone And Renin Activity Using Liquid Chromatography Tandem Mass Spectrometer (LC-MS/MS)**; DARYL HEE[1]; Yi Ting Tan[1]; *[1]Changi General Hospital, Singapore, Singapore*

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WP 199 **Evaluating CID and EAD Fragmentation for Improved Localization of Hydroxyl Radical Protein Footprinting (HRPF) Modifications**; Jiana Duan[1]; Emily Hart[1]; Remco Van Soest[2]; Zoe Zhang[2]; Haichuan Liu[2]; Scot Weinberger[1]; *[1]GenNext Technologies, Half Moon Bay, CA; [2]SCIEX, Redwood City, CA*

WP 200 **Data-Independent Acquisition As Tool For Quantitative Cross-linking Mass Spectrometry**; Zdenek Kukacka[1]; Valerie Prochazkova[1]; Petr Novak[1]; *[1]Institute of Microbiology CAS, Prague, Czech Republic*

WP 201 **FAST PHOTOCHEMICAL OXIDATION OF NUCLEIC ACIDS COUPLED TO HIGH-RESOLUTION MS ANALYSIS**; Marek Polak[1, 2]; Jiří Černý[3]; Daniel Kavan[2, 4]; Michael Volny[4, 5]; Petr Novak[2, 4]; *[1]Faculty of Science, Charles University, Prague, Czech Republic; [2]BioCeV – Institute of*

Microbiology, The Czech Academy of Sciences, Prague, Czech Republic; [3]*BioCev – Institute of Biotechnology, The Czech Academy of Sciences, Prague, Czech Republic;* [4]*Charles University, Prague 2, Czech Republic;* [5]*University of Chemistry and Technology, Prague, Czech Republic*

WP 202 **Astral vs. Exploris: Comparing the Identification of In-Cell Fast Photochemical Oxidation of Proteins Within HEK-293 Cells and PBMCs**; Jalah Morris[1]; Lisa M. Jones[1]; [1]*University of California San Diego, La Jolla, CA*

WP 203 **Optimizing data acquisition and analysis in cross-linking mass spectrometry on the Orbitrap Astral instrument**; Max Ruwolt[1]; Lars Muehlberg[1]; Yi He[2]; Diogo Borges Lima[1]; Rosa Viner[2]; Fan Liu[1, 3]; [1]*Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany;* [2]*ThermoFisher Scientific, San Jose, CA;* [3]*Charité, Universitätsmedizin Berlin, Berlin, Germany*

WP 204 **Probing epichaperome structure in mouse embryonic stem cells using native gel electrophoresis and a novel high-throughput in-gel crosslinking method**; Luke A Botticelli[1]; Seth McNutt[1]; Feixia Chu[1]; [1]*University of New Hampshire, Durham, NH*

WP 205 **Characterization of Antibody Binding Epitopes Using Carbene Chemical Footprinting and Electron Activated Dissociation**; Fan Zhang[1]; Haichuan Liu[2]; Benjamin Bell[1]; Remco van Soest[2]; Zoe Zhang[2]; Breanna Vollmar[1]; Shree Bhagwat[1]; Laurence Fayadat-Dilman[1]; Elliott Jones[2]; Jason Hogan[1]; [1]*Merck, South San Francisco, CA;* [2]*SCIEX, Redwood City, CA*

WP 206 **Covalent Labeling to Probe a Protein with an Intrinsically Disordered Domain**; Evan N Whitford[1, 2]; Philip C. Lacey[1, 2]; Elijah Day[1, 2]; Steffen Lindert[1, 2]; Vicki H. Wysocki[1, 2, 3]; [1]*Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH;* [2]*Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH;* [3]*Campus Chemical Instrumentation Center, The Ohio State University, Columbus, OH*

WP 207 **Fast photochemical oxidation of proteins for understanding proteoform differences implicated in racial health disparities associated with triple negative breast cancer**; Jorge Jacinto[1]; Lisa M. Jones[1]; [1]*University of California, San Diego, La Jolla, CA*

WP 208 **Comprehensive proteomic analysis of modulating proteins from calcium sensitive cells in circuits**; Alexandria S. Battison[1]; Jeremy Borniger[1]; Jeremy Balsbaugh[2]; [1]*Cold Spring Harbor Laboratory, Cold Spring Harbor, NY;* [2]*University of Connecticut Proteomics and Metabolomics Facility, Storrs, CT*

WP 209 **Probing the Interactions of IGF2 with the Entire Extracellular Region of CI-MPR using Hydroxyl Radical Protein Footprinting**; Sandeep K Misra[1]; Richard Bohnsack[2]; Nancy Dahms[2]; Joshua S Sharp[3]; [1]*University of Mississippi, Oxford, MS;* [2]*Medical College of Wisconsin, Milwaukee, WI;* [3]*UNIVERSITY OF Mississippi, Oxford, MS*

WP 210 **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[1]; Fiona L. Kearns[1]; Mac Kevin E. Braza[1]; Mia A. Rosenfeld[1]; Surl-Hee Ahn[2]; Rommie E. Amaro[1]; Lisa M. Jones[1]; [1]*UC San Diego, La Jolla, CA;* [2]*UC Davis, Davis, CA*

WP 211 **α-Methylene-β-Lactone Scaffold for Proteome-wide Capture of Biogenic Amine-Protein Interactions**; Clodette Punzalan[1]; Robert Jervine V Ortega[1]; Jose Intano Jr. [1]; Amy R Howell[1]; Xudong Yao[1]; [1]*University of Connecticut - Storrs, Storrs Mansfield, CT*

WP 212 **Evaluating effective reagents for tyrosine bioconjugation by mass spectrometry**; Sharel Cornelius[1]; Adway Ouseph Zacharias[1]; Saiful M Chowdhury[1]; [1]*University of Texas at Arlington, Arlington, TX*

WP 213 **Footprinting MS Elucidates the Binding Site of oligomeric Amyloid Beta with sTREM2**; Wesley J. Wagner[1]; Thomas J. Brett[2]; Michael L. Gross[1]; [1]*Washington University in St. Louis, St. Louis, MO;* [2]*Washington University School of Medicine, St. Louis, MO*

WP 214 **Novel mass spec-cleavable protein crosslinking agents for detecting direct residue-residue contacts**; Bjorn-Erik Wulff[1]; Joshua E. Elias[2]; Pehr A.B. Harbury[1]; [1]*Stanford University, Stanford, CA;* [2]*Chan Zuckerberg Biohub, San Francisco, CA*

WP 215 **Chemical and UV-mediated protein–DNA/RNA XL-MS used for establishing an inventory of DNA-/RNA-binding proteins in mitochondria**; Henri Göthert[1, 2]; Monika Raabe[1]; Aleksandar Chernev[1]; Juan Tasis Galarza[1]; Luis D Cruz-Zaragoza[3]; Peter Rehling[3]; Henning Urlaub[1, 2]; [1]*Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany;* [2]*Bioanalytics Group, Institute of Clinical Chemistry, University Medical Center Göttingen, Göttingen, Germany;* [3]*Department of Cellular Biochemistry, University Medical Center Göttingen, Göttingen, Germany*

WP 216 **Singlet oxygen may serve as a probe for protein footprinting**; Marek Polak[1]; Lukáš Fojtík[1, 2]; Jasmína Portašíková[1, 2]; Daniel Kavan[1, 2]; Petr Man[1, 2]; Michael Volny[2, 3]; Petr Novak[1, 2]; [1]*Institute of Microbiology of the Czech Academy of Sciences, Prague, Czech Republic;* [2]*Faculty of Science, Charles University, Prague, Czech Republic;* [3]*Institute of Microbiology of the Czech Academy of Sciences, 142 20, Prague, Czech Republic*

WP 217 **Why are crosslinking yields so low? Insights from click-based protein crosslinking**; Nicholas Brodie[1]; Bruno C Amaral[1]; Andrew RM Michael[1]; David C Schriemer[1]; [1]*University of Calgary, Calgary, AB*

WP 218 **DSBSO-based XL-MS Analysis of Breast Cancer PDX Tissues to Delineate Protein Interaction Network in Clinical Samples**; Fenglong Jiao[1]; Clinton Yu[1]; Wheat Andrew[1]; Lijun Chen[2]; Tung-Shing Mamie Lih[2]; Hui Zhang[2]; Lan Huang[1]; [1]*University of California Irvine, Irvine, CA;* [2]*Johns Hopkins University, Baltimore, MD*

WP 219 **Application of Methionine Oxidation Footprinting in Intact Proteins (MOFIP) to Mouse Brain**; Anju Teresa Sunny[1]; Kellye Cupp-Sutton[1]; Patrycja Szamweber[1]; Yanting Guo[2]; Laura-Isobel McCall[3]; Si Wu[1]; [1]*University of Alabama, Tuscaloosa, AL;* [2]*University of Oklahoma, Norman, OK;* [3]*San Diego State University, San Diego, CA*

WP 220 **Triangulating Protein Interactions: Expanding Proteomic Insights with Three-Site Cross-Linking**; Clinton Yu[1]; Xiaorong Wang[1]; Eric Novitsky[1]; Paul Morenkov[1]; Scott Rychnovsky[1]; Lan Huang[1]; [1]*University of California, Irvine, Irvine, CA*

WP 221 **Silyl Ether Enables High Coverage Chemoproteomic Interaction Site Mapping**; Chau Ngo; *University of California Los Angeles, Los Angeles, CA*

WP 222 **Binding Efficency Analysis of PEGylated Aptamers by LC-MS**; Cole D. Babcock[1, 2]; Makan Golizeh[1]; [1]*Concordia University of Edmonton, Edmonton, AB;* [2]*Babcocks Synthetics Ltd., Wainwright, AB*

WP 223 **Computational Approach to Understanding Nitrile Imines as Photocrosslinkers in Gas-Phase Peptide Scaffold Ions**; Kim Vu[1]; Hongyi Zhu[1]; František Tureček[1]; [1]*University of Washington, Seattle, WA*

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WP 224 **An exploration of novel electrophiles in the context of a living cell using an Inverse Drug Discovery approach**; Sarah M Norman[1]; Zhen Li[1]; Leonard Yoon[1]; Jin-Quan Yu[1]; Jeff W Kelly[1]; [1]*Scripps Research Institute, San Diego*

WP 225 **Rapid Point-of-Care Quantitative Analysis of HIV Medications using Two-Dimensional Tandem Mass Spectrometry (2D MS/MS)**; Yanyang Hu[1]; Joseph V. Caruso[1]; Peter L. Anderson[2]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN;* [2]*University of Colorado Denver, Aurora, CO*

WP 226 **Development and Optimization of an LC-MS/MS Quantitation Method for Drug Analysis in Bovine Rumen**; Ludmyla Santos Tavares[1]; Raymond Zielinski[1]; [1]*Zoetis Inc., Kalamazoo, MI*

WP 227 **Improvement of mass spectrum output for separation and determination of chiral compounds by 2D LC and UPC2 systems**; Xiaopeng Wu[1]; Xiaoxia Yang[1]; Peiyun An[1]; Jinlian Lu[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

WP 228 **The timsTOF Ultra enables deep global ubiquitinomics of ultra-low protein input samples for validating degrader drug targets**; Philipp Strohmidel[1]; Martin Steger[2]; Uli Ohmayer[2]; Björn Schwalb[2]; Torsten Mueller[1]; Christian Albers[1]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]NEOsphere Biotechnologies GmbH, Planegg, Germany*

WP 229 **Dual polarity, high-resolution Acoustic Ejection Mass Spectrometry for high-throughput library screening in 1536-well plates**; David Calabrese[1]; Nate Hoxie[1]; Zina Itkin[1]; Meghav Verma[1]; John Janiszewski[1]; Jonathan Shrimp[1]; Kelli Wilson[1]; Sam Michael[1]; Matthew D Hall[1]; Lyle Burton[2]; Tom Covey[2]; Chang Liu[2]; *[1]NIH/NCATS, Rockville, Maryland; [2]SCIEX, Concord, ON*

WP 230 **Determination of a Cucurbit[7]uril (CB[7])–PEG Conjugate in Dog Plasma and Rat Plasma by LC-MS/MS**; Qing Chang[1]; Man Yang[1]; Yanfu Ren[1]; Zhiyu Li[2]; Lili Xing[2]; Yi Tao[2]; Liang Shen[2]; *[1]WuXi AppTec, Suzhou, China; [2]WuXi AppTec, Shanghai, China*

WP 231 **A high-throughput screening platform to probe protein/metabolite interactions enables rapid discovery of functional allosteric binding sites for drug discovery**; Joseph Lapointe[1]; Olga Zurita[1]; Trisha Moro[1]; Gordon Murray[1]; Kaitlyn Selmer[1]; Christopher F Bennett[1]; Melissa J Buskes[1]; Anil Padyana[1]; Maria-Jesus Blanco[1]; Shomit Sengupta[1]; Marion Dorsch[1]; Thomas Roddy[1]; *[1]Atavistik Bio, Cambridge, MA*

WP 232 **Comprehensive Host Cell Protein Analysis and Viral Protein Identification in AAV Samples Using Optimized Wide Window Acquisition Method**; Shihan Huo[1]; Song Nie[1]; Yongzheng Cong[1]; Shunhai Wang[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Inc., Tarrytown, NY*

WP 233 **Triple Quadrupole Infrared Matrix-Assisted Laser Desorption Electrospray Ionization Mass Spectrometry for Faster Scans**; James Sawicki[1]; Andrew Radosevich[2]; Fan Pu[3]; Charles Maxey[4]; Alexander Buzenski[3]; Timothy Brayman[3]; Chankdika Amarasinghe[4]; Nari Talaty[3]; Omprakash Nacham[3]; John Shanley[3]; David Chang-Yen[3]; Nathaniel Elsen[3]; Eloy R. Wouters[4]; Jon D Williams[3]; *[1]Abbvie, North Chicago, IL; [2]AbbVie, Inc., North Chicago, IL; [3]AbbVie Inc., North Chicago, IL; [4]ThermoFisher Scientific, San Jose, CA*

WP 234 **Bioanalytical Characterization and Stability Evaluation of Drug Metabolites in Biological Matrices - A Case Study**; Yongliang (Kevin) Zhang[1]; Georgia Cornelius[1]; Kosea Frederick[2]; Petia Shipkova[1]; France Landry[1]; *[1]Bristol Myers Squibb, Lawrenceville, NJ; [2]Bristol Myers Squibb, Cambridge, MA*

WP 235 **Stereoselective Protein-Probe Reactivity of Fluorotriazines: An Inverse Drug Discovery Exploration**; Karina Nugroho[1]; Gabriel M. Kline[1]; Christian M. Cole[1]; Jeffery W. Kelly[1]; *[1]Scripps Research, La Jolla, CA*

WP 236 **Innovative orthogonal method for Host Cell Protein characterization combining Immuno-affinity enrichment and MS Analysis**; Noelia De Lama[1, 2]; Diego Bertaccini[3]; Christine Carapito[1, 2]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, IPHC (UMR 7178), CNRS, Strasbourg, France; [2]Infrastructure Nationale de Protéomique ProFI – FR2048, Strasbourg, France; [3]Global Analytical Development, Merck KGaA, Darmstadt, Germany*

WP 237 **Micro-scale ubiquitin-remnant peptide enrichment and MS analysis on the timsTOF Ultra for protein degrader target validation**; Martin Steger[1]; Uli Ohmayer[1]; Björn Schwalb[1]; Henrik Daub[1]; *[1]NEOsphere Biotechnologies GmbH, Planegg, Germany*

WP 238 **Structure and Dynamics of Glutide Therapeutics Analyzed by Native Mass Spectrometry and Ion Mobility**; Syuan-Ting Kuo[1]; Zhenyu Xi[1]; Xin Yan[1]; David H Russell[1]; *[1]Texas A&M, College Station, TX*

WP 239 **Comparative Analysis of Recalled Metformin Using SIFT-MS and Liquid Chromatography**; Anthony Qualley[1]; Mark J. Perkins[2]; Vaughan S. Langford[3]; Colin J. Hastie[2]; *[1]Syft Technology, Pittsburgh, PA; [2]Element Lab Solutions, Cambridge, United Kingdom; [3]Syft Technologies, Christchurch, New Zealand*

WP 240 **Multiomics Analysis of the Lipoxygenase Inhibitor, Utreloxastat, a New Therapeutic Targeting Ferroptosis** ; Arba Karcini[1]; Jenna R Mattice[1]; Anna C Krieger[1]; Whitney Lobo[1]; Yuting Mao[2]; Jana Narasimhan[2]; Marla Weetall[2]; Angela Minnella[1]; Jeff Trimmer[1]; Joey C Latham[1]; *[1]PTC Therapeutics, Inc., Mountain View, CA; [2]PTC Therapeutics, Inc., Bridgewater, NJ*

WP 241 **A LC–MS/MS method for the evaluation of cystic fibrosis mucus permeability of drug candidates targeting the Aryl Hydrocarbon Receptor**; Lorenzo Sardelli[1]; Enrica Frasca[1]; Olga Valentina Garbero[1]; Alex Africano[1]; Claudio Medana[1]; Sonja Visentin[1]; *[1]University of Turin, Torino, Italy*

WP 242 **Evaluating selectivity, mechanism of action, and efficacy of KT-253, a heterobifunctional MDM2 degrader**; Charles Lincoln Howarth[1]; Min Yuan[1]; Christina Kolodzy[1]; Sarah Martinez[1]; Eric Kuhn[1]; Yogesh Chutake[1]; Joyoti Dey[1]; Nancy Dumont[1]; Douglas Shorten[1]; Juliet Williams[1]; Susanne B Breitkopf[1]; Kirti Sharma[1]; *[1]Kymera Therapeutics, Watertown, MA*

WP 243 **Heterobifunctional Degrader KT-333 Inhibits Tumor Growth by Induction of Selective Ubiquitination of Lysine Residues on the Surface of STAT3**; Dirk M Walther[1]; Yatao Shi[1]; Christopher M Browne[1]; Caroline Daigle[1]; Xue Fei[1]; Kiran Mahasenan[1]; Anand Ramanathan[1]; Sarah Martinez[1]; Susanne B Breitkopf[1]; Eric Kuhn[1]; Joyoti Dey[1]; Kirti Sharma[1]; *[1]Kymera Therapeutics, Watertown, MA*

WP 244 **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[1]; Haiting Zhang[2]; *[1]Regeneron, Tarrytown, NY; [2]Regeneron Pharmaceuticals, Tarrytown, NY*

WP 245 **Multiplexed Biomarker Quantitation Using Parallel Reaction Monitoring (PRM) LC-MS/MS Coupled with FAIMS and the Newomics DuoESI Source**; Keely E. Fuller[1]; Yuehe Ding[2]; Phillip Y. Chu[1]; Jianhui Zhu[2]; Mandy Kwong[1]; Daojing Wang[3]; Jonathan L Josephs[1]; John C. Tran[1]; Chengjie Ji[2]; Rachel Liuqing Shi[1]; *[1]Genentech Inc, South San Francisco, CA; [2]NovaBioAssays, Boston, Massachusetts; [3]Newomics Inc., Berkeley, CA*

WP 246 **Developing Improved Intact Protein LC/MS Workflows for the Analysis and Quantitation of Adeno-Associated Viral Capsids**; Alyssa Nodland[1]; Roxana Eggleston-Rangel[1]; Michael McGinley[1]; *[1]Phenomenex, Torrance, CA*

WP 247 **Small Fragment Screening Targeting Stromal Cell Death and Cysteine Activity Mapping in Keratoconus Pathology using TMT-MS**; Xinyue Liu[1]; Ka Yang[1]; Joao A. Paulo[1]; Edward L. Huttlin[1]; Steven P. Gygi[1]; *[1]Harvard Medical School, Boston, MA*

WP 248 **Multiomics analysis post fluorescence-activated cell sorting – a cautionary tale**; Feroza K. Choudhury[1]; Viji Premkumar[1]; Jana Zecha[1]; Jonathan Boyd[1]; Andrew S. Gaynor[2]; Zengli Guo[3]; Tom Martin[4]; Raffaello Cimbro[5]; Erik L. Allman[1]; Sonja Hess[1]; *[1]Dynamic Omics, Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD; [2]Oncology Cell Therapy, ICC, Oncology R&D, AstraZeneca, Gaithersburg, MD; [3]Biologics Engineering, Cell Therapeutics & Viral Technologies, AstraZeneca, Gaithersburg, MD; [4]Biologics Engineering, Oncology TTD, ADC, AstraZeneca, Gaithersburg, MD; [5]Dynamic Omics, Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Cambridge, United Kingdom*

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WP 249 **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[1, 2]; Angelina Jaeger[1, 2]; Haley Tomlin[3]; Jamieson Atkinson[3]; Chris G Gill[1, 2, 4, 5]; Erik T Krogh[1, 2]; [1]*Vancouver Island University, Nanaimo, BC;* [2]*University of Victoria, Victoria, BC;* [3]*British Columbia Conservation Foundation, Nanaimo, BC;* [4]*Simon Fraser University, Burnaby, BC;* [5]*University of Washington, Seattle, WA*

WP 250 **Detection, Quantification, and Isomer Differentiation of Per- and Polyfluoroalkyl substances (PFAS) using MALDI-TOF with Trapped Ion Mobility**; Aidan J Reynolds[1]; Abby M. Smith[1]; Tian Autumn Qiu[1, 2]; [1]*Department of Chemistry, Michigan State University, East Lansing, Michigan;* [2]*MSU Center for PFAS Research, East Lansing, Michigan*

WP 251 **The Physical and Chemical Characterization of Levitated Microparticles using a Linear Quadrupole Coupled to Electrospray Mass Spectrometry**; Stephanie Salas[1]; Ravleen Kaur Kohli[1]; James F. Davies[1]; [1]*University of California, Riverside, Riverside, CA*

WP 252 **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[1]; Eemeli Eronen[1]; Marko Mäkinen[1]; Janne Jänis[1]; [1]*University of Eastern Finland, JOENSUU, Finland*

WP 253 **Advanced Nontargeted High Resolution Mass Spectrometry Techniques for Revealing Missing Disinfection Byproducts**; Nicholas J. P. Wawryk[1]; Tingting Zhao[2]; Qiming Shen[1]; Tao Huan[2]; Xing-Fang Li[1]; [1]*University of Alberta, Edmonton, AB;* [2]*University of British Columbia, Vancouver, BC*

WP 254 **Advanced Nontarget Characterization of Amine-containing Compounds in Suwannee River Standard Reference Materials**; Qiming Shen[1]; Nicholas J. P. Wawryk[1]; Tingting Zhao[2]; Di Zhang[1]; Kristin Carroll[1]; Tao Huan[2]; Xing-Fang Li[1]; [1]*University of Alberta, Edmonton, AB;* [2]*University of British Columbia, Vancouver, BC*

WP 255 **Rapid, Direct Screening of Priority Metal Contaminants in Environmental Systems with a Reactive 3D-Printed Cone Spray Ionization Methodology**; Jonathan N. Chilaka[1]; Ebenezer H. Bondzie[1]; Jamie R. Wieland[1]; Christopher Hamaker[1]; Patrick W. Fedick[2]; Christopher Mulligan[1]; [1]*Illinois State University, Normal, IL;* [2]*Naval Air Warfare Center, Weapons Division (NAWCWD), China Lake, CA*

WP 256 **Speciation of Algae geneses using Matrix-Assisted Laser Desorption Ionization to Build a Mass Spectra Database**; Cheyenne D Copling[1]; Kevin R Tucker[2]; Joao Nail[2]; Carolyn Butts-Willmsmeyer[2]; [1]*Southern Illinois University of Edwardsville, Edwardsville, IL;* [2]*Southern Illinois University Edwardsville, Edwardsville, IL*

WP 257 **Detailed characterization of urinary arsenic metabolic profiles with simultaneous elemental and molecular mass spectrometry**; Tetiana Davydiuk[1]; Jagdeesh S. Uppal[1]; Xiufen Lu[1]; Ahsan Habib[2]; Brandon L. Pierce[2]; Jennifer A. Graydon[3]; Megan Reichert[3]; X. Chris Le[1]; [1]*University of Alberta, Edmonton, AB;* [2]*University of Chicago, Chicago, IL;* [3]*Alberta Health, Health Protection Branch, Edmonton, AB*

WP 258 **Analysis of Volatile Organic Compounds (VOCs) in Water using Headspace-GCMS in Accordance with US EPA Method 8260D**; Elvi Horiyanto[1]; Chun Kiang Chua[1]; Elgin Guo Wei Ting[1]; Cynthia Lahey[1]; [1]*Shimadzu AP, Singapore, Singapore*

WP 259 **Probing Anthropogenic Pollution Profiles of Coastal Ecosystems Through Public Non-Targeted Tandem Mass Spectrometry Data**; Jarmo-Charles Julian Kalinski[1, 2]; Abzer Kelminal Pakkir Mohamed Shah[3]; Shane Farrell[4]; Lisa Schellenberg[5, 6]; Andreas F. Haas[5]; Rosemary A. Dorrington[2]; Daniel Petras[1, 7]; [1]*College of Natural and Agricultural Sciences, University of California Riverside, Riverside, CA;* [2]*Department of Biochemistry and Microbiology, Rhodes University, Makhanda, South Africa;* [3]*Functional Metabolomics Lab, Cluster of excellence CMFI, University of Tuebingen, Tuebingen, Germany;* [4]*Bigelow Laboratory for Ocean Sciences, East Boothbay, ME;* [5]*Department of Marine Microbiology and Biogeochemistry, Royal Netherlands Institute for Sea Research (NIOZ), Texel, Netherlands;* [6]*Institute for Biodiversity and Ecosystem Dynamics (IBED), University of Amsterdam, Amsterdam, Netherlands;* [7]*University of Tuebingen, CMFI Cluster of Excellence, Interfaculty Institute of Microbiology and Infection Medicine, Tübingen, Germany*

WP 260 **LC/MS quantitative aspects of GenX: impact of pH on dimer formation**; Joshua Shipman[1]; Eduard Rogatsky[1]; [1]*Mosaic Diagnostics, Overland Park, KS*

WP 261 **Environmental characteristics, exposures, and oxidative potentials of emerging contaminants of para-phenylenediamine quinones**; Zongwei Cai[1]; Wei Wang[1]; Guodong Cao[1]; [1]*Hong Kong Baptist University, Kowloon Tong, Kowloon, Hong Kong*

WP 262 **Ion mobility mass spectrometry reveals fluorotelomer ethoxylates in indoor dust and industrial wastewater**; Karl Jobst[1]; Katherine L. Steeves[2]; Meera J. Bissram[2]; Sonya Kleywegt[3]; Douglas Stevens[4]; Frank L. Dorman[5]; Andre J. Simpson[6]; Myrna J. Simpson[6]; Lindsay S. Cahill[2]; [1]*Memorial University Of Newfoundland, St. John's, NL;* [2]*Memorial University of Newfoundland, St. John's, NL;* [3]*Ontario Ministry of the Environment, Conservation and Parks, Toronto, ON;* [4]*Waters, Milford, MA;* [5]*Waters Corporation, Milford, MA;* [6]*University of Toronto, Toronto, ON*

WP 263 **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 264 **Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous Matrices Using EPA Method 533 with Automated Solid Phase Extraction (SPE)**; Renee N.G Huang[1]; Thuy Nguyen[1]; Surjit Saini[1]; [1]*Valley Water, San Jose, California*

WP 265 **Multiple Tools for Demanding Needs: Trace Detection of Organochlorine Pesticides by Agilent 7000E and 7010C GC/MS/MS**; Erinn M ONeill[1]; Alexis Willey[1]; Anastasia Andrianova[1]; [1]*Agilent Technologies, Wilmington, DE*

WP 266 **Characterizing the chemical composition of ultrafine particles from non-tailpipe emissions using the thermal desorption chemical ionization mass spectrometer**; Madeline Cooke[1]; Adam E. Thomas[1]; Véronique Perraud[1]; Lisa M. Wingen[1]; Paulus S. Bauer[1]; Michelia Dam[1]; Barbara J. Finlayson-Pitts[1]; James N. Smith[1]; [1]*University of California, Irvine, Irvine*

WP 267 **Chemical ionization mass spectrometry analysis of low volatility vapors emitted from automotive braking**; Adam E. Thomas[1]; Madeline E. Cooke[1]; Michelia Dam[1]; Véronique Perraud[1]; Lisa M. Wingen[1]; Michael J. Ezell[1]; Paulus S. Bauer[1]; Barbara J. Finlayson-Pitts[1]; James N. Smith[1]; [1]*University of California, Irvine, Irvine, CA*

WP 268 **Development of targeted and non-targeted methods for quantitative and qualitative analysis of per- and polyfluoroalkyl substances in biosolids and biochars**; Emir Nazdrajic[1]; Arthur E. Lee[1]; Joshua Cullen[2, 3]; Javier Ordonez-Loza[4, 5]; J. Larry Campbell[1, 6, 7]; Kati Bell[8]; Naomi Klinghoffer[4, 5]; Franco Berruti[4, 5]; W. Scott Hopkins[1, 6, 9]; [1]*University of Waterloo, Waterloo, ON;* [2]*University of Western Ontario, London , ON ;* [3]*Institute for Chemicals and Fuels from Alternative Resources, Ilderton, ON;* [4]*University of Western Ontario, London, Ontario;* [5]*Institute for Chemicals and Fuels from Alternative Resources, Ilderton, Ontario;* [6]*Watermine Innovation, Waterloo, ON;* [7]*Bedrock Scientific Inc, Milton, ON;* [8]*Brown and Caldwell, Nashville, TN;* [9]*Centre for Eye and Vision Research, Hong Kong, Hong Kong*

WP 269 **Chemical and structural characterization of organic aerosol emitted from laboratory burning of Boreal and Arctic peat by 21T FT-ICR MS**; Eric Schneider[1, 2]; Christopher P. Rüger[1, 2]; Anika Neumann[1, 2]; Martha L. Chacón-Patiño[3]; Markus Somero[4]; Meri Ruppel[5]; Mika

Ihalainen[4]; Kajar Köster[4]; Olli Sippula[4]; Hendryk Czech[1, 6]; Ralf Zimmermann[1, 6]; *[1]Department of Analytical Chemistry, University Rostock, Rostock, Germany; [2]Department Life, Light & Matter, University Rostock, Rostock, Germany; [3]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [4]Department of Environmental and Biological Sciences, University of Eastern Finland, Kuopio, Finland; [5]Atmospheric Composition Unit, Finnish Meteorological Institute, Helsinki, Finland; [6]Joint Mass Spectrometry Centre, Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Munich, Munich, Germany*

WP 270 **Identification and quantification of atmospherically relevant organic peroxides in secondary organic aerosol**; Markus Kalberer; *University of Basel, Basel, Switzerland*

WP 271 **Using a Compact Single Quadrupole LC-MS for PFAS Analysis**; Kathleen K Luo[1]; Om K Shrestha[1]; Megan P Davis[1]; Landon A Wiest[1]; Evelyn H Wang[1]; Michelle Zipse[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

WP 272 **LC-MS/MS analysis ofcomprehensive PFAS including EPA method 1633 list and ultrashort chain PFAA**; Tanya Napolitano; *Shodex, New York, NY*

WP 273 **Expanding the LC-MS Workflow to Analyze Ultrashort-chain PFAS Analytes in Aqueous Environmental Samples**; Erika P Portero[1]; Ana Ramos[1]; Lam Leung[1]; *[1]The Chemours Company, Newark, DE*

WP 274 **Probing sub-10nm nanoparticles chemical composition from reactions of methanesulfonic acid with multifunctional amines using thermal desorption chemical ionization mass spectrometry**; Veronique Perraud[1]; Paulus S. Bauer[2]; Patricia M. Morris[1]; Kanuri Roundtree[1]; Cathy Wong[1]; James N. Smith[1]; Barbara J. Finlayson-Pitts[1]; *[1]UC Irvine, Irvine, CA; [2]UC Irvine, Irvine*

WP 275 **Online Membrane Sampling coupled to ESI-MS for rapid quantification of toxic components in Oil Sands Process-Affected Waters**; Dylan Steenis[1, 2]; Joseph Monaghan[1, 2]; Ian Vander Meulen[3, 4]; Josh Baker[5]; John Headley[4]; Chris G Gill[1, 2, 6, 7]; Erik T Krogh[1, 2]; *[1]Vancouver Island University, Nanaimo, BC; [2]University of Victoria, Victoria, BC; [3]University of Saskatchewan, Saskatoon, SK; [4]Environment Canada, Saskatoon, SK; [5]Nautilus Environmental, Burnaby, BC; [6]Simon Fraser University, Burnaby, BC; [7]University of Washington, Seattle, WA*

WP 276 **Enhancing LC-MS Strategies for the Characterization and Attribution of AFFF Samples with SLIM-Enabled High-Resolution Ion Mobility**; Thomas Lubinsky[1]; Michelle English[1]; Frederick Strathmann[1]; *[1]MOBILion Systems, Chadds Ford, PA*

WP 277 **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 278 **Quantification of 8 chlorination Disinfectant byproducts (DBPs) from water using liquid-liquid extraction and Gas Chromatography with Mass Spectrometry**; Jessin Mathai[1]; Shailesh Damale[2]; Anant Lohar[2]; *[1]Shimadzu, Dubai, United Arab Emirates; [2]Shimadzu Middle East and Africa FZE, Dubai, United Arab Emirates*

WP 279 **Exploring honey bee exposome using a novel passive sampler together with low- and high-resolution mass spectrometry: the case of Denmark**; María Murcia-Morales[1]; Francisco José Díaz-Galiano[1]; María Del Mar Gómez-Ramos[1]; José Luis Oller-Serrano[1]; Cristian Valderrama Conca[1]; Jozef J. M. Van Der Steen[2]; Flemming Vejsnæs[3]; Amadeo R. Fernández-Alba[1]; *[1]Chemistry and Physics Department, University of Almeria, Agrifood Campus of International Excellence (ceiA3), Almería, Spain; [2]Alveus AB Consultancy, Oisterwijk, Netherlands; [3]Danish Beekeepers Association, Fulbyvej, Sorø, Denmark*

WP 280 **Non-targeted screening of unknown per- and polyfluoroalkyl substances in cosmetics and human plasma using ion mobility-mass spectrometry**; Chloe Penney[1]; Xiaolei Li[1]; Roshanak Amiri[1]; Atanu Sarkar[1]; Karl Jobst[1]; *[1]Memorial University of Newfoundland, St. John's, NL*

WP 281 **Developing a method to monitor the estrogen-inducible proteins in fishes from the Great Lakes upon exposure to environmental contaminants**; Krishan S Weraduwage[1]; Taniya M Jayaweera[1]; Bernard Crimmins[2]; Sujan Fernando[2]; Thomas M Holsen[2]; Costel C Darie[1]; *[1]Biochemistry and Proteomics Laboratories, Department of Chemistry and Biomolecular Science,Clarkson University, Potsdam, NY; [2]2 Department of Civil and Environmental Engineering, Clarkson University, Potsdam, NY*

WP 282 **Utilization of Automated Solvent Extraction with a Triple Quadrupole Mass Spectrometer following EPA Method 1633 for PFAS Analysis in Soil**; Landon A Wiest[1]; Om K Shrestha[1]; Benedict Liu[2]; Kathleen K Luo[1]; Megan Davis[1]; Evelyn H Wang[1]; Alicia Stell[2]; Ruth Marfil-Vega[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]CEM Corporation, Matthews, NC*

WP 283 **A single and straightforward method for VOCs analysis: Water quality analysis**; Ricardo Tamashiro Reis[1]; Ana Caroline Martimiano[1]; Isabela de Oliveira e Silva[1]; Rodrigo Ossamu Saga Kitamura[1]; *[1]Shimadzu do Brasil, Barueri, Brazil*

WP 284 **Development of a LCMS Methodology to Characterize and Quantitate Fluorinated Compounds in Consumer Product**; Michael Deible[1]; Logan Miller[2]; Rachel Hale[1]; William Lipps[2]; *[1]RJ Lee Group, Pittsburgh, Pennsylvania; [2]Shimadzu Scientific Instruments, Columbia, MD*

WP 285 **Reversed Phase Separation Improvements for Short Chain PFAS**; Conner McHale[1]; Barry Boyes[1]; Charles Powley[2]; *[1]Advanced Materials Technology, Wilmington, DE; [2]Center for PFAS Solutions, New Castle, DE*

WP 286 **Development of a Non-target HRMS Approach for Microcystin Analysis to Bridge the Gap Between ELISA and LC-MS/MS**; Jonathan Zapata[1]; Matthew Prescott[1]; *[1]Metropolitan Water District, La Verne, CA*

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WP 287 **Fragment correlation mass spectrometry of multi-charged ions to improve molecular structural identification and resolve complex mixtures**; Yangjie Li[1]; Guy Cavet[2]; Richard N Zare[1]; Taran Driver[1]; *[1]Stanford University, Stanford, CA; [2]Flatiron Bio, LLC, Palo Alto, CA*

WP 288 **Square Parametric Excitation in a Digital Linear Ion Trap**; Grace O Capek[1]; Etienne Garand[1]; *[1]University of Wisconsin - Madison, Madison, WI*

WP 289 **To separate or not to separate: MS/MS fragmentation-based uncoupling of bile acid regio- and stereoisomers**; Ipsita Mohanty[1]; Yasin El Abiead[1]; Lee R. Hagey[1]; Pieter C. Dorrestein[1]; *[1]University of California San Diego, La Jolla, CA*

WP 290 **Overcoming artefacts in Fourier transform-isotope ratio mass spectrometry for low abundance isotopocules**; Nils Kuhlbusch[1, 2]; Konstantin Aizikov[3]; Dmitry Grinfeld[2]; Dmitry Strelnikov[2]; Issaku E. Kohl[2]; Dieter Juchelka[2]; Alexander A. Makarov[2, 4]; Heiko Hayen[1]; Andreas Hilkert[2]; *[1]University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermofisher, Bremen, Germany; [4]Utrecht University, Utrecht, Netherlands*

WP 291 **Additively Manufactured Quadrupole Mass Filter Yields Competitive RGA Performance for a Fraction of the Production Cost**; Colin Eckhoff[1]; Luis F. Velasquez-Garcia[1]; *[1]MIT, Cambridge, MA*

WP 292 **Sub-optimal conditions for enzymatic cleavage - A way to achieve maximum protein sequence coverages**; Dirk Dobritzsch[1]; Matthew A. Fuszard[1]; *[1]Martin-Luther-University Halle-Wittenberg, Halle, Germany*

WP 293 **Chiral Recognition by Mass Spectrometry with the Combinations of Two Chiral Selectors**; Qi Yi; *Hong Kong Polytechnic University, Kowloon, Hong Kong*

WP 294 **Reproducibility analysis of clinically-relevant targets identifies durable phosphopeptide ions**; Andrew Williamson[1]; Amy E Campbell[2]; Janet Kelsall[3]; Luis Nobre[3];

Pedro Moreno-Cardoso[3]; Weronika S Borek[3]; David N Perkins[3]; David J Britton[3]; Arran D Dokal[3]; *[1]Kinomica, Macclesfield, United Kingdom; [2]Kinomica Ltd, Macclesfield, United Kingdom; [3]Kinomica Ltd, Macclesfield, Cheshire, United Kingdom*

WP 295 **Photochemical vapor generation: a tool for analyte introduction in inductively coupled plasma mass spectrometry**; Daniel LG Borges; *Federal University of Santa Catarina, Florianopolis, Brazil*

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WP 296 **Site-Specific N-Glycosylation of Glycoproteins in Influenza Vaccines – A Study of Variability**; Zachary C Goecker[1]; Meghan C Burke[1]; Concepcion A Remoroza[1]; Yi Liu[1]; Yuri A Mirokhin[1]; Sergey L Sheetlin[1]; Dmitrii V Tchekhovskoi[1]; Xiaoyu Yang[1]; Stephen E Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

WP 297 **Studying the effects of glycosylation on the entry of SARS-CoV-2 using high-mass MALDI-MS**; Yuye Zhou[1, 2]; Congrui Tan[1]; Renato Zenobi[1]; *[1]ETH Zurich, Zurich, Switzerland; [2]KTH Royal Institute of Techonology, Stockholm, Sweden*

WP 298 **A Chemoenzymatic Method for Site-Specific Profiling of Protein O-GlcNAcylation**; Longping Fu[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

WP 299 **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[1]; Christopher Mullen[1]; Roberto Gamez[1]; Ping F. Yip[2]; Rosa Viner[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Lexington, MA*

WP 300 **Profiling the glycocode of CD24 using a combined mass spectrometry approach**; Tim S. Veth[1]; Kayla A. Markuson[2]; Nicholas M. Riley[2]; *[1]University of Washington, Seattle, WA; [2]University of Washingon, Seattle, WA*

WP 301 **The role of N-glycans in SARS-CoV-2 Spike protein structure and cellular receptor/antibody binding**; Sarah H Osman[1]; John R. Barr[1]; Dongxia Wang[1]; *[1]CDC, Chamblee, GA*

WP 302 **Characterization of offline fractionation methods for in-depth glycoproteomics**; Ruby Zhang[1]; Kayla A. Markuson[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA*

WP 303 **Enhanced surface accessibility of SARS-CoV-2 Omicron spike protein due to an altered glycosylation profile**; Dongxia Wang[1]; Zijian Zhang[2]; Jakub Baudys[1]; Christopher Haynes[1]; Sarah H. Osman[1]; John R Barr[1]; James Gumbart[2]; *[1]Centers of Disease Control and Prevention (CDC), Atlanta, GA; [2]Georgia Tech, Atlanta, GA*

WP 304 **Tracing labeled metabolites in hypothermic CHO cells reveals a role in affecting secreted mAb quality**; Xin Bush[1]; Nicholas Trunfio[1]; Erica Berilla[1]; Casey Kohnhorst[1]; Nicole Azer[1]; Roberta King[2]; David Naoki Powers[1]; *[1]FDA, Silver Spring, MD; [2]University of Rhode Island, Kingston, RI*

WP 305 **XIC-centric analysis recovers glycopeptide spectra missed by database searches**; Guanghui Wang[1]; Zheng Zhang[1]; Yi Liu[1]; Meghan C Burke[1]; Sergey L Sheetlin[1]; Stephen E Stein[1]; *[1]NIST, Gaithersburg, MD*

WP 306 **Glycopeptide Libraries of Human Plasma Glycoproteins**; Yi Liu[1]; Meghan C Burke[1]; Sergey Sheetlin[1]; Goecker C Zachary[1]; Zheng Zhang[1]; Yuxue Liang[1]; Guanghui Wang[1]; Yuri A Mirokhin[1]; Xiaoyu Yang[1]; Dmitrii V Tchekhovskoi[1]; Stephen E Stein[1]; *[1]NIST, Gaithersburg, MD*

WP 307 **Bottom-up glycoprotein analysis workflows including column switching, Differential Mobility Spectrometry, Electron Activation Dissociation and Ultraviolet Photodissociation**; Charlotte Jacquet[1]; Gérard Hopfgartner[1]; *[1]University of Geneva, Geneva, Switzerland*

WP 308 **Workflow Development and Optimization for Proteomic and Glycoproteomic Analysis of Platelets**; Ying Sheng[1]; Yunlong Zhao[1]; Yuan Mao[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY*

WP 309 **Utilizing novel EAD QTOF technology for bioactive protein characterization**; Greg Roman[1]; Dilip Reddy[2]; Zhengwei Chen[2]; Xiaoning Lu[3]; Lei Xiong[4]; *[1]Sciex, Framingham, MA; [2]SCIEX, USA, Framingham, MASSACHUSETTS; [3]Helainia, New York, New York; [4]SCIEX, Redwood City, CA*

WP 310 **Characterization of the N- and O-Glycosylation of Recombinant Mpox E8 Viral Protein**; Jakub Baudys[1]; Theodore R. Keppel[1]; Yu Zhou[1]; John R. Barr[1]; Dongxia Wang[1]; *[1]Centers of Disease Control and Prevention (CDC), Atlanta, GA*

WP 311 **Global O-glycoproteome enrichment and analysis enabled by a robust combinatorialenzymatic workflow**; Rohit Budhraja[1]; Taewook Kang[1]; Jinyong Kim[1]; Neha Joshi[1]; Kishore Garapati[1]; Akhilesh Pandey[1]; *[1]Mayo clinic, Rochester, MN*

WP 312 **Cognitive Decline in Older Adults with Type 2 Diabetes: Unraveling Site-Specific N-linked Mass Spectrometry Based Glycoproteomic Alterations**; Yishai Levin[1]; David Morgenstern[1]; Hila Wolf Levy[1]; Barak Markus[1]; Itzik Cooper[2]; Michal Schnaider Beeri[3]; *[1]Weizmann Institute of Science, Rehovot, Israel; [2]Sheba Medical Center, Tel Hashmer, Israel; [3]Rutgers University, New Brunswick, NJ*

WP 313 **An Innovative Approach for Examining Disease-Related N-Glycopeptides in Small Extracellular Vesicles: A Case Study on Traumatic Brain Injury**; Ayobami O. Oluokun[1]; Mojibola O Fowowe[1]; Cristian D Gutierrez-Reyes[1]; Moyinoluwa Adeniyi[1]; Sherifdeen B Onigbinde[1]; Oluwatosin E Daramola[1]; Angel J Garcia[1]; Firas Kobeissy[2]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA*

WP 314 **Ionization Efficiency of Homologous Saccharides in various Modes of Electrospray**; Nicholas Allen[1]; Ian T Ferraro[1]; Nancy Fernandes[2]; Thaddaeus Webster[2]; Carrie Mason[2]; Tolulope Ogunsanya[1]; Anyin Li[1]; *[1]University of New Hampshire, Durham, NH; [2]Lonza Biologics, Portsmouth, New Hampshire*

WP 315 **Detection of Glucose-Regulated Sites of Protein O-GlcNAc Modification**; Lauren E Ball[1]; Mi-Hye Lee[1]; Jennifer R Bethard[1]; Rony Hull[1]; Susana Comte-Walters[1]; Mauricio J Reginato[2]; *[1]Medical University of South Carolina, Charleston, SC; [2]Drexel University, Philadelphia, PA*

WP 316 **Simultaneous Deglycosylation and Nontryptic Protease Digestion**; Jade K. Macdonald[1]; Richard R. Drake[1]; Anand S. Mehta[1]; Peggi Angel[1]; *[1]Medical University of South Carolina, Charleston, SC*

WP 317 **Network method for building a sample-specific glycan database for N-linked glycosylation from MS/MS data**; Aliana Tang[1]; Marshall W. Bern[2]; *[1]Piedmont High School, Piedmont, CA; [2]Protein Metrics, LLC, Cupertino, CA*

WP 318 **High-Throughput Spatial Glycoproteomics: Deciphering Age-Related Glycosylation Changes in the Mouse Brain**; Delf-Magnus Kummerfeld[1, 2]; Johanna Schrader[3]; Aleksander J. Nowak[4]; Joanna M. Kirkpatrick[4]; Peter Milland[5]; Eugen Damoc[4]; Boris V. Skryabin[2]; Hans H. Wandall[6]; Timofey S. Rozhdestvensky[2]; Sergey Y. Vakhrushev[6]; *[1]Leibniz Institute on Aging - Fritz Lipmann Institute (FLI), Jena, Germany; [2]Transgenic animal and genetic engineering Models (TRAM), Core facility, Medical Faculty, Muenster University, Muenster, Germany; [3]L3S Research Center, Hannover, Germany; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [5]Thermo Fisher Scientific, Bremen, Germany; [6]University of Copenhagen, Department of Cellular and Molecular Medicine, Copenhagen Center for Glycomics, Copenhagen N, Denmark*

WP 319 **Differential N-Glycosylation Site Occupancy Depends on Distinct Amino Acid Sequence Features of Oligosaccharyltransferase and Acceptor Polypeptides**; Marium Khaleque[1]; Amanda Nouwens[2]; Elisa Fadda[3]; Benjamin Schulz[2]; *[1]Columbia University, New York, NY;*

[2]University of Queensland, Brisbane, Australia; [3]Maynooth University, Kildare, Ireland

WP 320 **Large Scale Characterization of N-linked Glycopeptides from Human Serum Using Hilic Enrichment and LC-MS Analysis**; Raghavendra Rao Pasupuleti[1]; Jonathan C Trinidad[1]; *[1]Department of Chemistry, Indiana University, Bloomington, IN, 47405*

WP 321 **Determination of Glycoform Masses of SARS-CoV-2 Spike Protein Variants by Electron Capture Charge Reduction Mass Spectrometry**; Zhixin Xu[1, 2]; Chen Du[1, 2]; Eduardo Olmedillas[3]; Regina M. Edgington[1]; Sophie R. Harvey[2]; Erica Ollmann Saphire[3, 4]; Vicki H. Wysocki[1, 2]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH; [3]Center for Vaccine Innovation, La Jolla Institute for immunology, La Jolla, California; [4]Department of Medicine, University of California, San Diego, La Jolla, California*

WP 322 **Analyzing Patterns of Sugar Fragmentation from Glycopeptide Tandem Mass Spectra**; Jonathan C. Trinidad[1]; Gabriel D Newton[1]; *[1]Indiana University Bloomington, Bloomington, IN*

WP 323 **Method Development for Ferret IgG N-Glycosylation Profiling from serum using timsTOF Pro2**; Thao T. Nguyen[1]; Min Hui Guan[1]; Lei Li[2]; Brian P. Mooney[1]; Michael C. Greenlief[1]; Xiu Feng Wan[1]; *[1]University of Missouri-Columbia, Columbia, MO; [2]Georgia State University, Atlanta, GA*

WP 324 **Identifying Protein Carriers of α2,3 sialylated N-linked glycosylation using bioorthogonal derivatization and enrichment**; Hongxia Bai[1]; Peggi M Angel[1]; Richard R Drake[1]; *[1]Medical University of South Carolina, Charleston, SC*

WP 325 **Intact Glycopeptide Analysis of Human Colon Cancer Tissue by High Resolution Liquid Chromatography-Tandem Mass Spectrometry**; Kathryn L. Kapp[1, 2]; Fernando J. Garcia Marques[1]; Abel Bermudez[1]; Nikhiya Shamsher[1]; Scot Liu[3]; Jeong Kim[3]; Ashok Dongre[4]; Sharon J. Pitteri[1]; *[1]Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; [2]Propel Postdoctoral Scholars Program, Stanford University School of Medicine, Stanford, CA; [3]Bristol Myers Squibb, Redwood City, CA; [4]Bristol Myers Squibb, Cambridge, MA*

WP 326 **Alternative glycoprotein labeling to access the intact cell surface proteome**; Emmajay Sutherland[1]; Nicholas M. Riley[1]; *[1]Department of Chemistry, University of Washington, Seattle, WA*

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WP 327 **Improving sensitivity of acoustic-ejection mass spectrometry in biological matrices using solid-phase extraction and carrier solvent optimization**; Md Jahangir Alam[1]; Grace Proske[1]; Bernard K Choi[1]; Rajesh Desai[1]; Paul Harradine[1]; *[1]Merck & Co. Inc., West Point, PA*

WP 328 **Capillary-flow sub-minute gradient LC/MS/MS for robust and ultrahigh-speed proteomics**; Ayana Tomioka[1]; Ryota Tomioka[1]; Eisuke Kanao[1, 2]; Kosuke Ogata[1]; Koshi Imami[3]; Naoyuki Sugiyama[1]; Yasushi Ishihama[1, 2]; *[1]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; [2]National Institutes of Biomedical Innovation, Health and Nutrition, Ibraki, Japan; [3]RIKEN Center for Integrative Medical Sciences, Yokohama, Japan*

WP 329 **High-throughput Mass Spectrometry (HTMS) Techniques for Bile Salt Export Pump (BSEP) Assay**; Jie Li[1, 2]; Nicolás Morato[2]; Lori Westover[3]; Pravien Abeywickrema[3]; Jieping Geng[3]; Madison Piassek[3]; David Harden[3]; Iulia Strambeanu[1]; Nico Vervoort[4]; Bo Hao[1]; Karel Goossens[4]; Zhicai Shi[1]; Harsha Gunawardena[5]; Juncai Meng[3]; R. Graham Cooks[2]; *[1]Global Discovery Chemistry, Janssen R&D, Spring House, PA; [2]Department of Chemistry, Purdue University, West Lafayette, IN; [3]Discovery Technology and Molecular Pharmacology, Janssen R&D, Spring House, PA; [4]CPRD, Janssen R&D, Beerse, Belgium; [5]Cell Engineering & Analytical Sciences, Janssen R&D, Spring House, PA*

WP 330 **Quality control system and QC data analysis pipeline for high throughput targeted LC-MS proteomics encompassing sample quality to instrument suitability**; Jonathan T Bui[1]; Chi D. L. Nguyen[1]; Erika Hernandez[1]; Dragana Noe[1]; Zachary Dwight[1]; Jennifer E. Van Eyk[2]; Susan Mockus[1]; *[1]Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA; [2]Advanced Clinical BioSystems Research Institute, Cedars-Sinai Medical Center, Los Angeles, CA*

WP 331 **Comparing plate-based high-throughput proteomics approaches for plasma depletion: antibody-based resin vs perchlorate precipitation**; Nathan Hendricks[1]; Josselin Ortiz[1]; Angel Keoseyan[1]; Santosh D Bhosale[1]; Annie Moradian[1]; Susan Mockus[1]; *[1]Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, California*

WP 332 **Characterization of Complex Cellular Signatures from Organophosphate Exposure Over Time Using Integrated Multiomic Analysis**; Tara Harvey[1, 2]; Emilio S. Rivera[1, 2]; Emilia A. Solomon[2]; Claire K. Sanders[3]; Joshua D. Breidenbach[1, 2]; Kes A. Luchini[1, 2]; Grace M. Thornhill[1, 2]; Brett R. Blackwell[1, 2]; Chi-Yen Tseng[1, 2]; Erick S. LeBrun[1, 2]; Marc Alvarez[2]; Abigale S Mikolitis[1, 2]; Bob Williams[2]; Zachary J. Sasiene[1, 2]; Ethan M. McBride[1, 2]; Austin R. Anderson[1, 2]; Lauren K. Heine[1, 2]; Jessica A. Salguero[1, 2]; Francisca E. Rodriguez[1, 2]; Salvator J. Palmisano[1, 2]; Phillip M. Mach[1, 2]; Trevor G. Glaros[1, 2]; *[1]Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [2]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [3]Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM*

WP 333 **Rapid Discovery of Medical Countermeasures against Emerging Pathogens using High-throughput DESI and 2D MS/MS**; Dalton Snyder[1]; Andrew Eller[1]; Scott Griffin[1]; Megan Guetzloff[1]; Miranda Jacobs[1]; Ann Donnelly[1]; Andrew Houvenagle[1]; Kevin Rosenbaum[1]; Austin Stieglitz[1]; Ilya Shinkeyev[1]; Kerry O'Donnell[1]; Brandon Reese[1]; Anna Leech[1]; Mitch Wells[1]; *[1]Teledyne FLIR, West Lafayette, IN*

WP 334 **HT-Intact Covalent Binding: Analysis automation workflow for scaled multiplexed screening with stringent quality control**; Matthew Green[1]; Juan Florez[2]; Stephan Heyse[2]; Stephen Steigele[2]; *[1]Genedata, Cambridge, United Kingdom; [2]Genedata, Basel, Switzerland*

WP 335 **High-throughput Acoustic Ejection Mass Spectrometry with adjustable signal durations**; Bradley Schneider[1]; Jing Ma[2]; Chiu Cheong Aw[2]; Heguang Ji[2]; Lin Shuxian[2]; Xuejiao Yin[2]; Huiyin Tey[2]; Chang Liu[1]; *[1]SCIEX, Concord, ON; [2]SCIEX, Singapore, Singapore*

WP 336 **Automated online protein-ligand binding and its detection using native mass spectrometry**; Weijing Liu[1]; Wilson Phung[2]; Wendy Sandoval[2]; Rosa Viner[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Genentech Inc, South San Francisco, CA*

WP 337 **Life in the Fast Lane: A Rapid Screening Method for the SAMHSA Urine and Oral Fluid Drug Lists by RapidFire-MS**; Jennifer Cottine Hitchcock; *Agilent Technologies, Santa Clara, CA*

WP 338 **Automated and High Throughput Analysis of AAV Biotherapeutics Using SampleStream and Individual Ion Mass Spectrometry**; Samuel E. Janisse[1]; Mike Goodwin[2]; Ryan T. Fellers[1]; Ping F. Yip[2]; Kristina Srzentic[3]; Kyle P. Bowen[2]; Josh Smith[4]; Jonathan Bones[4]; Michael W. Senko[2]; Jared O. Kafader[1]; Philip D. Compton[5]; Neil L. Kelleher[1]; *[1]Proteomics Center of Excellence, Northwestern University, Evanston, Illinois; [2]ThermoFisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Reinach, Switzerland; [4]National*

Institute for Bioprocessing Research and Training, Dublin, Ireland; [5]Integrated Protein Technologies, Inc, Evanston, IL

WP 339 **Systematic Comparison of High-Throughput Activity-Based Proteomics LC-MS Methods for Quantitative Reactive Cysteinome Profiling in a Cellular Context**; Violette Gautier[1]; Giada Marino[2]; Nagarjuna Nagaraj[2]; Pierre-Olivier Maux[3]; Marion Tondeur[1]; Guillaume Vink[1]; Marie Guillemot[1]; Navratan Bagwan[1]; Philipp Strohmidel[4]; Catherine Pech[5]; Francois Autelitano[1]; *[1]EVOTEC, Toulouse, France; [2]Evotec München GmbH, Munich, Germany; [3]Evotec SE, Toulouse, France; [4]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [5]EVOTEC, Toulouse, France*

WP 340 **Fine-tuning Mag-Net: Advancing plasma proteome profiling through parameter optimization and comparative analysis**; Adele Nel[1, 2]; Sindisiwe Buthelezi[3]; Ireshyn S Govender[1]; Previn Naicker[1, 3]; Andrea Ellero[1, 2]; Stoyan Stoychev[4]; Justin Jordaan[1]; Christine Wu[5]; Michael J. MacCoss[6]; *[1]ReSyn Biosciences, Pretoria, South Africa; [2]University of Pretoria, Pretoria, South Africa; [3]Council for Scientific and Industrial research, Pretoria, South Africa; [4]ReSyn BioSciences, Johannesburg, South Africa; [5]University of Washington, seattle, WA; [6]University of Washingon, Seattle, WA*

WP 341 **Evaluation of Improved Methodology for Proteograph XT Nanoparticle-Enriched Plasma with ThermoFisher Orbitrap Astral Mass Spectrometer**; Lee S Cantrell[1]; Eltaher Elgierari[1]; Jian Wang[1]; Gabriel Castro[1]; Ryan W. Benz[1]; Jimmy Zeng[2]; Bruce Wilcox[2]; Serafim Batzoglou[1]; *[1]Seer Inc., Redwood City, CA; [2]Prognomiq Inc., San Mateo, California*

WP 342 **High-throughput and rapid screening of PFAS in drinking water using solid-phase microextraction with microfluidic open interface-mass spectrometry**; MALVIKA DUTT[1, 2]; WEI ZHOU[2]; ACHILLE CAPPIELLO[1, 3]; JANUSZ PAWLISZYN[2]; *[1]UNIVERSITY OF URBINO CARLO BO, URBINO, Italy; [2]University of Waterloo, Waterloo, ON; [3]Vancouver Island University, Nanaimo, BC*

WP 343 **A proximity proteomics pipeline for subcellular proteome and protein interaction mapping**; Xiaofang Zhong[1]; Qiongyu Li[1]; Benjamin Polacco[1]; Trupti Patil[1]; Aaron Marley[1]; Helene Foussard[1]; Prachi Khare[1]; Rasika Vartak[1]; Jiewei Xu[1]; Jeffrey DiBerto[2]; Bryan Roth[2]; Manon Eckhardt[1]; Mark Von Zastrow[1]; Nevan Krogan[1]; Ruth Huttenhain[1]; *[1]University of California-San Francisco, San Francisco, CA; [2]University of North Carolina at Chapel Hill, Chapel Hill, NC*

WP 344 **Development of a High-Throughput Screening Assay to Identify Inhibitors of Plasmodium falciparum Acetyl-CoA synthetase Using RapidFire Mass Spectrometry**; De Lin[1]; Andrew Plater[1]; Joao Pisco[1]; Avinash Punekar[1]; Andrew Shepherd[1]; Sharon Shepherd[1]; Leah Torrie[1]; Beatriz Baragana[1]; David W. Gray[1]; *[1]Drug Discovery Unit, School of Life Sciences, University of Dundee, Dundee, United Kingdom*

WP 345 **Desorption Electrospray Ionization and 2D-MS/MS for High Throughput Biomolecular Analysis**; Thomas C. Sams[1]; Louis Edwin Gonzalez[1]; Sam Edward Ying[1]; Christina R. Ferreira[1]; Kai-Hung Huang[1]; Nicolás Morato[1]; Kitmin Chen[1]; Eric Dziekonski[1]; Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN*

WP 346 **Accelerated Late-Stage Functionalization of Opioid Drugs in Microdroplets**; Jyotirmoy Ghosh[1]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN*

WP 347 **A novel tandem LC workflow for proteome analysis with near 100% MS utilization**; Runsheng Zheng[1]; Martin Rendl[1]; Tabiwang N Arrey[2]; Neloni Wijeratne[3]; Christopher Pynn[1]; Alec Valenta[1]; Ece Aydin[1]; Maksim Daniliuk[4]; Robert van Ling[5]; Scott M Peterman[3]; Eugen Damoc[2]; Claudia Martins[3]; Philip Remes[3]; Cristina Jacob[3]; Wim Decrop[1]; Martin Samonig[1]; Anne Morgenstern[1]; *[1]Thermo Fisher Scientific, Germering, Germany; [2]Thermo Fisher Scientific GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, Vilnius, Lithuania; [5]Thermo Fisher Scientific, Breda, Netherlands*

WP 348 **Accelerating Drug Discovery and Lead Optimization: Unleashing the Power of High Throughput Mass Spectrometry for Rapid Molecular Insights**; Patrick Bingham[1]; Karen Maegley[1]; Juliana Piscatelli[1]; John Lazzaro[2]; Brendon Kapinos[2]; Jamie Tourville[2]; Alandra Quinn[2]; Nallely Juarez-Rodriguez[2]; *[1]Pfizer Inc., San Diego, CA; [2]Pfizer Inc., Groton, CT*

WP 349 **A Chemical Derivatization MRM Method for High-Throughput MS-Based Screening to Identify Small-Molecule Modulators of Deoxyhypusine Synthase**; Christopher A LeClair[1]; Dingyin Tao[1]; Yuhong Fang[1]; Ken Chih-Chien Cheng[1]; Wei Zhao[1]; Ravi Tharakan[1]; Shyh-Ming Yang[1]; Myung-Hee Park[2]; Matthew D Hall[1]; *[1]National Center for Advancing Translational Sciences, NIH, Rockville, MD; [2]National Institute of Dental and Craniofacial Research, NIH, Bethesda, MD*

WP 350 **High throughput online buffer exchange native MS method for screening of protein-ligand interactions**; Mohamed Ibrahim Gadallah[1]; Jada N. Walker[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

WP 351 **High-throughput Mass Spectrometry - Based Detec--tion of Deamination Activity of ADAR1 without Prior Separation**; Yating Wang[1]; Travis Pemberton[1]; Ping Zhang[2]; Iyoncy Rodrigo[2]; Zhigang Wang[1]; *[1]Bristol Myers Squibb, Cambridge, MA; [2]Bristol Myers Squibb, Lawrenceville, NJ*

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WP 352 **Gel-assisted mass spectrometry imaging enables sub-micrometer spatial lipidomics**; Yat Ho Chan[1]; Koralege C Pathmasiri[1]; Dominick Pierre-Jacques[1]; Nannan Tao[2]; Joshua L. Fischer[2]; Ethan Yang[2]; Stephanie Cologna[1]; Ruixuan Gao[1]; *[1]University of Illinois Chicago, Chicago, IL; [2]Bruker Daltonics, Billerica, MA*

WP 353 **Multiplexed Quantitative Imaging of Proteins Delivered by Polymeric Nanocarriers**; Teerapong Jantarat[1]; Dheeraj K. Agrohia[1]; Ritabrita Goswami[1]; Yağız Anıl Çiçek[1]; Vincent M. Rotello[1]; Richard W. Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

WP 354 **Decellularization improves MALDI-MS Imaging of Extracellular Matrix Proteins in Tissues**; Akaansha Rampal[1]; Ngoc Vu[1]; Shelly R. Peyton[1]; Richard W. Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

WP 355 **Imaging mass spectrometry of sulfatide isomers enabled by gas-phase charge inversion ion/ion reactions**; Julia R Bonney[1, 2]; Ariana E Stratton[1]; Yingchan Guo[1]; Paul Zerebinski[1]; Boone M. Prentice[1]; *[1]University of Florida Department of Chemistry, Gainesville, FL; [2]Department of Neurosurgery, Brigham and Women's Hospital, Harvard Medical School, Boston, MA*

WP 356 **3D Mass Imaging of Bacterial Biofilm Composition using Water Cluster SIMS**; Mark Duncan Mills[1]; Naoko Sano[1]; Michal Ryszka[1]; Kate McHardy[1]; David Ward[1, 2]; Nick A. Von Jeinsen[1, 2]; *[1]Ionoptika, Chandlers Ford, United Kingdom; [2]Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom*

WP 357 **Cryo-3D MSI for Plant cells at 90 Kelvin by Water Cluster Secondary Ion Mass Spectrometry (Cluster SIMS)**; Michal Ryszka[1]; Naoko Sano[1]; Mark Duncan Mills[1]; Paul Blenkinsopp[1]; *[1]Ionoptika Ltd, Chandlers Ford, United Kingdom*

WP 358 **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[1]; Yunxin Ouyang[2]; Tatiana Segura[2]; David C. Muddiman[1]; *[1]North Carolina State University, Raleigh, NC; [2]Duke University, Durham, NC*

WP 359 **Novel quantitative mass spectrometry imaging strategy using the method of standard addition**; Lucie Davidová[1]; Ingela Lanekoff[1]; *[1]Uppsala University, Uppsala, Sweden*

WP 360 **Hight efficiency mass spectrometry imaging using single-pixel imaging stratergy**; Aojie Zhang[1]; Xiangyu Guo[1]; Wenpeng Zhang[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China*

WP 361 **Enhancing Analytical Precision: Method Optimization for Robust Peptide MALDI-MSI Analysis**; Jessica K Lukowski[1]; Jaenyeon Kim[2]; Young Ah Goo[2]; *[1]Washington University School of Medicine, St Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

WP 362 **Development of Standard Materials for MALDI MS Imaging of Tissue N-glycans and Applications to Glycosylation Dysregulation in Multiple Sclerosis**; Xuan Lan Mai[1]; Bozena Szulc[1]; William Branton[1]; Ling Han[1]; Elena N. Kitova[1]; Christopher Power[1]; Jason Plemel[1]; Lara K. Mahal[1]; John S. Klassen[1]; *[1]University of Alberta, Edmonton, AB*

WP 363 **MALDI Mass Spectrometry Imaging Analysis of Gene expression and Metabolomic Signatures in Alzheimer's Disease Model**; Kyle A Vanderschoot[1]; Jacob P. Padilla[1]; Kelli A. Steinneman[1]; Jacopo Di Lucente[1]; Izumi Maezawa[1]; Lee-way Jin[1]; Marie C. Heffern[1]; Elizabeth K Neumann[1]; *[1]University of California, Davis, Davis, California*

WP 364 **On-tissue dataset-dependent MALDI-TIMS-MS2 bioimaging**; Steffen Heuckeroth[1, 2]; Arne Behrens[3]; Carina Wolf[2]; Arne Fütterer[3]; Ansgar Korf[1]; Henning Richter[4]; Astrid Jeibmann[5]; Uwe Karst[2]; Robin Schmid[6]; *[1]mzio GmbH, Bremen, Germany; [2]University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]University of Zurich, Zürich, Switzerland; [5]Institue for Neuropathology, University of Muenster, Muenster, Germany; [6]Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic*

WP 365 **Parallel data acquisition for multiplexed mass spectrometry imaging targeting oxidized cholesterol metabolites in multiple sclerosis**; Varun Vashneel Sharma[1]; Gabor Toth[1]; Johan Lillja[1]; Cathrin Hansen[2]; Gijs Kooij[2]; Ingela Lanekoff[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Amsterdam University Medical Center, Amsterdam, Netherlands*

WP 366 **A novel MALDI IMS approach for improved spatial visualization of small molecules in formalin-fixed paraffin-embedded tissue sections**; Georgia Charkoftaki[1]; Athina Lisgara[1]; Alvaro Santos-Neto[1, 2]; Reza Aalizadeh[1]; Michael Becker[3]; Nina Gonnella[4]; Vladimir V Papov Jr. [4]; Vasilis Vasiliou[1]; *[1]Yale School of Public Health, New Haven, CT; [2]University of São Paulo, São Carlos, Brazil; [3]Boehringer Ingelheim, Biberach an der Riß, Germany; [4]Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, Connecticut*

WP 367 **The effect of solvents on metabolomic and lipidomic recovery from formalin-fixed paraffin-embedded human brain tissue sections by DESI-MSI**; Tassia Venga Mendes[1]; Emily Xinlei Ma[2]; Patrick R. Hof[3]; Dan Meyer[4]; Samantha Abate[4]; Elizabeth McDonough[4]; Merina Varghese[3]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Houston, TX; [2]Rice University, Houston, TX; [3]Icahn School of Medicine at Mount Sinai, New York, NY; [4]GE HealthCare, Niskayuna, NY*

WP 368 **Cyclic MALDI-IHC for Successive High-plex and Multimodal Imaging of Tissues and Tissue Microarrays**; Leonardo G. Dettori[1]; Gargey Yagnik[1]; Philip Carvalho[1]; Mark J. Lim[1]; Kenneth J. Rothschild[1, 2]; *[1]AmberGen Inc., Billerica, MA; [2]Boston University, Department of Physics and Photonics Center, Boston, MA*

WP 369 **Tuning MSI for Deeper Spatial Proteomics in Drug Discovery: Matrix Enhancing Charge State and Search Algorithm Design for IM-MS Bias**; Emily R. Sekera[1]; Xusheng Wang[1]; Yingxue Fu[1]; Anthony High[1]; Zoran Rankovic[1]; John J. Bowling[1]; *[1]St. Jude Children's Research Hospital, Memphis, TN*

WP 370 **Optimization of liquid extraction surface analysis (LESA) for microenvironments within Pseudomonas aeruginosa biofilms**; Dharmeshkumar Parmar[1, 2]; Abigail Weaver[3]; Joshua D Shrout[3, 4]; Jonathan V Sweedler[1, 2]; *[1]Department of Chemistry, University of Illinois Urbana-Champaign, Champaign, IL; [2]Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Champaign, IL; [3]Department of Biological Sciences, University of Notre Dame, Notre Dame, Indiana; [4]Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, Notre Dame, Indiana*

WP 371 **Mass spectrometry imaging detection of counterfeits and forgery**; Veronika Tibljas[1]; Robert Bradshaw[1]; Simona Francese[1]; Marjory Da Costa Abreu[1]; *[1]Sheffield Hallam University, Sheffield, United Kingdom*

WP 372 **Combination of fluorescence and IR images with protein and lipid MALDI Imaging allows more insights into disease phenotypes**; Corinna Henkel[1]; Bjoern Wendik[1]; Tanja Bien[1]; Bram Heijs[1]; Arne Behrens[1]; David Ahlers[2]; Jan Schwenzfeier[3]; Tobias Boskamp[1]; Soeren-Oliver Deininger[1]; Jens Christmann[4]; Uwe Karst[2]; Jens Soltwisch[3]; Andrea Tannapfel[4]; Savannah Snyder[5]; Katherine A. Stumpo[5]; *[1]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; [2]Institute of Inorganic and Analytical Chemistry, University of Münster, Münster, Germany, Münster, Germany; [3]Institute of Hygiene, University of Münster, Münster, Germany, Münster, Germany; [4]Institute for Pathology, Ruhr-University Bochum, Bürkle-de-la-Camp-Platz 1, 44789 Bochum, Germany, Bochum, Germany; [5]Bruker Scientific, LLC, Billerica, MA*

WP 373 **MALDI-imaging of tryptic peptides: Improvements in spatial resolution in mammalian tissue and first applications in plants and ecotoxicological model organisms**; Bastian Jahreis[1]; Julia Kokesch-Himmelreich[1]; Oliver Wittek[1]; Andreas Römpp[1]; *[1]Chair of Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany*

WP 374 **Enhancing a Statistics-Based System Suitability Testing Approach for Mass Spectrometry Imaging with Improved Sampling Methods and a Diverse Analyte Panel**; Quinn Mills[1]; Russell R Kibbe[1]; Alexandria L. Sohn[1]; Emily C Hector[2]; Andrew J Percy[3]; Krista Backiel[3]; David C. Muddiman[1]; *[1]North Carolina State University, Raleigh, NC; [2]Department of Statistics, North Carolina State University, Raleigh, NC; [3]Cambridge Isotope Laboratories, Tewksbury, Massachusetts*

WP 375 **Combining metabolite imaging mass spectrometry with multiplex confocal immunofluorescence microscopy for a multi-modal lymphoid tissue analysis pipeline**; Benjamin L. Oyler[1]; Adam Molyvdas[1]; Jeferson A. Valencia-Dávila[1]; Bindesh Shrestha[2]; Constantinos Petrovas[3]; Amina Woods[1]; Richard Koup[1]; *[1]NIH, Gaithersburg, MD; [2]Waters Corporation, Milford, Massachusetts; [3]University of Lausanne, Lausanne, Switzerland*

WP 376 **Sublimated/annealed aminated cinnamic acid analogues for high sensitivity 3 µm spatial resolution MALDI IMS of lipids in human tissues**; Martin Dufresne[1]; David M. G. Anderson[1]; Lukasz Migas[2]; Cody R Marshall[1]; Katerina V Djambazova[1]; Richard M. Caprioli[1]; Raf Van De Plas[2]; Jeffrey M Spraggins[1]; *[1]Vanderbilt University, Nashville, TN; [2]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands*

WP 377 **Metabolome profiling of mammalian tissue using varied mass spectrometry techniques for confident spatial identification**; Rosalie Chu[1]; Marija Velickovic[1]; Dusan Velickovic[1]; William Kew[1]; Karl K. Weitz[1]; Tujin Shi[1]; Tao Liu[1]; *[1]PNNL, Richland, WA*

WP 378 **Multimodal Omics Imaging of Human Brain Using MALDI HiPLEX-IHC**; Yumiko Toyama[1]; Takashi Nirasawa[2]; Shigeo Murayama[3]; Yuko Saito[3]; Maho Morishima[3]; Masaya Ikegawa[4]; *[1]Doshihsha University, Kyotanabe Kyoto, Japan; [2]Bruker Japan K.K., Yokohama, Japan; [3]The Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology,, Tokyo, Japan; [4]Doshisha University, Kyoto, Japan*

WP 379 **MnM: Co-spatial tissue imaging using MALDI and MIBI**; Davide G. Franchina[1]; Marc Bosse[1]; Sam Kimmey[2]; Michael Angelo[1]; Sean Bendall[1]; *[1]Stanford School of Medicine, Palo Alto, CA; [2]Ionpath, Menlo Park, CA*

WP 380 **Hybrid Imaging Analyses of Brain Tissue: Toward the Brain Atlas of Molecules, Elements and Metals**; Tadayuki Ogawa[1]; Eisei Tanaka[2]; Shino Takeda-Homma[3]; Takafumi Hirata[2]; Tomonari Umemura[4]; *[1]Dokkyo Medical University, Mibu-machi, Japan; [2]The University of Tokyo, Bunkyo-ku, Japan; [3]National Institute of Quantum Science and Technology, Inage, Japan; [4]Tokyo University of Pharmacy and Life Science, Hachioji, Japan*

WP 381 **MALDI Imaging of Lipids using Long-chain n-Alkyl Primary Ammonium and Conventional Matrix Conjugate Base Organic Salt Matrices**; Brandy Perkins[1]; Taylar Bell[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

WP 382 **Protocol for quantitative mass spectrometry imaging applied to samples with spatial heterogeneity**; Reza Shariatgorji[1]; Anna Nilsson[1]; Michael Niehues[1]; Tina Angerer[1]; Per Svenningsson[2]; Per E. Andren[3]; *[1]Uppsala university, Uppsala, Sweden; [2]Karolinska Institutet, Stockholm, Sweden; [3]Uppsala University, Uppsala, Sweden*

WP 383 **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[1]; Masato Hoshino[2]; Yumiko Toyama[1]; Takashi Nirasawa[3]; Yuko Saito[4]; Shigeo Murayama[4]; Masaya Ikegawa[1]; *[1]Doshisha University, Kyoto, Japan; [2]Japan Synchrotron Radiation Research Institute (JASRI/SPring-8), Hyogo, Japan; [3]Bruker Japan K.K., Yokohama, Japan; [4]The Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology,, Tokyo, Japan*

WP 384 **Design of a Novel Velocity-selected Spatial Map Ion Imaging Mass Spectrometer using SIMION**; Eric J Smoll Jr[1]; David W. Chandler[1]; Brian D Patterson[1]; Chrisopher J Kliewer[1]; *[1]Sandia National Labs, Livermore, CA*

WP 385 **Evaluation of ocular distribution of low molecular drug in mouse by MALDI mass spectrometry imaging**; Hiroyuki Yokoi[1]; Yasuhiro Takeji[2]; Takeshi Fukuhara[2]; Ryo Doyama[2]; Takumi Yasuno[1]; Masakazu Shibata[1]; Yosuke Kaneko[1]; *[1]Otsuka Pharmaceutical Co., Ltd, Tokushima City, Japan; [2]Otsuka Pharmaceutical Co., Ltd, Minoh City, Japan*

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WP 386 **Enhancing Proteoform Characterization in Top-Down Mass Spectrometry Using Internal Fragment Ions**; Arthur Grimaud[1]; Masa Babovic[1]; Frederik Haugaard Vrdlovec Holck[1]; Ole Nørregaard Jensen[1]; Veit Schwämmle[1]; *[1]University of Southern Denmark, Odense, Denmark*

WP 387 **Quantifying proteoforms in bottom-up proteomics data using tree-based quantification**; Constantin Ammar[1]; Marvin Thielert[1]; Eugenia Voytik[1]; Caroline Weiss[1]; Edwin Rodriguez[1]; Maximilian T. Strauss[2]; Florian Rosenberger[1]; Wen-Feng Zeng[1]; Matthias Mann[1]; *[1]Max Planck Institute of Biochemistry, Planegg, Germany; [2]Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark*

WP 388 **QuavaProt: Prediction of Variant Peptide for Screening and Quantitation via Mass Spectrometry**; Constantinos Blidjios[1]; Yassene Mohammed[2, 3, 4]; Pallab Bhowmick[2]; Vincent R. Richard[2]; Christoph H. Borchers[2, 4, 5, 6]; *[1]Department of Oncology, McGill University, Montreal, QC; [2]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [3]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [4]Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; [5]Division of Experimental Medicine, McGill University, Montreal, QC; [6]Department of Pathology, McGill University, Montreal, QC*

WP 389 **Development of a novel Sf9 database for monitoring host cell proteins (HCPs) on Sf9-derived adeno-associated viruses (AAVs)**; Josh Smith[1]; Marina Ainciburu[1]; Ioanna Tzani[1]; Aaron Richardson[1]; Michelle Chain[1]; Sara Carillo[1]; Eugen Damoc[2]; Colin Clarke[1, 3]; Jonathan Bones[1, 3]; *[1]The National Institute for Bioprocessing Research & Training, Dublin, Ireland; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland*

WP 390 **proteoDA: an R package for quantitative proteomics**; Charity Washam[1]; Duah Alkam[1]; Allen Gies[1]; Kalyani Dhusia[1]; Michael Robeson, II[1]; Stephanie Byrum[1]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR*

WP 391 **From CsoDIAq to zoDIAq: Applying computer science coding standards to a complete python DIA-MS proteomic data analysis software**; Caleb Cranney[1]; Alexandre Hutton[1]; Jesse Meyer[1]; *[1]Cedars-Sinai Medical Center, Los Angeles*

WP 392 **Performance of LPGF Protein Validation in diverse sample types and mass spectrometry workflows**; Pedro Navarro[1]; Waqas Nasir[1]; Kai Fritzemeier[1]; Gorka Prieto[2]; Víctor M Guerrero-Sánchez[3]; Jesús Vázquez[3]; Christoph Henrich[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Department of Communications Engineering, University of the Basque Country (UPV/EHU), Bilbao, Spain; [3]Centro Nacional de Investigaciones Cardiovasculares Carlos III (CNIC), Madrid, Spain*

WP 393 **Improving Protein Identification Utilizing Various Chromatographic Methods and Multiple Search Engines**; Jesus D Castano[1, 2]; Francis Beaudry[1, 2]; *[1]Département de Biomédecine Vétérinaire, Faculté de Médecine Vétérinaire, Université de Montréal, Montréal, Quebec; [2]Centre de recherche sur le cerveau et l'apprentissage (CIRCA), Université de Montréal, Montréal, Quebec*

WP 394 **TopDIA: Proteoform Identification by Top-Down Data-Independent Acquisition Proteomics**; Abdul Rehman Basharat[1]; Xingzhao Xiong[2]; Tian Xu[3]; Yong Zang[4]; Liangliang Sun[3]; Xiaowen Liu[2]; *[1]Indiana University Purdue University Indianapolis, Indianapolis, IN; [2]Tulane University, New Orleans, LA; [3]Michigan State University, Department of Chemistry, East Lansing, MI; [4]Indiana University School of Medicine, Indianapolis, IN*

WP 395 **Protein identification based on Embedding Vectors Searching**; Leiver Campeon[1]; Sebastián Franco Gómez[1]; Mihira Kasun[1]; Lalin Theverapperuma[1]; Andi Krupke[1]; *[1]Expert Intelligence, Santa Clara, CA*

WP 396 **A Novel Real-Time Computational Assessment of Protein Differential Expression During Mass Spectrometry Experiments for Optimization of Data Acquisition**; Aarthie Senathirajah[1]; Yun-En Chung[1]; Amit Scheer[1, 2]; Jonathan R. Krieger[3]; Tharan Srikumar[3]; Daniel Figeys[1]; Theodore J. Perkins[1, 4]; Mathieu Lavallée-Adam[1]; *[1]University of Ottawa, Ottawa, ON; [2]Harvard University, Cambridge, MA; [3]Bruker Ltd., Milton, ON; [4]Ottawa Hospital Research Institute, Ottawa, ON*

WP 397 **ProteoSynth: A Tool for Ground Truth Benchmarking of Proteomics Data Processing Pipelines**; Matthew N. Dailey[1]; Dmitry Avtonomov[1]; Eric Kim[1]; Chris Wilkins[1]; Stefanie Kairs[1]; Sangtae Kim[1]; *[1]Bertis Bioscience, SAN DIEGO, CA*

WP 398 **Ab-Twister: Fast and accurate de novo sequencing of monoclonal antibodies**; Kira Vyatkina; *Sechenov University, Moscow, Russian Federation*

INFORMATICS: WORKFLOW AND DATA MANAGEMENT
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WP 399 **The PRIDE Crosslinking resource: Improving FAIR data practices for crosslinking datasets**; Suresh Chanaka Hewapathirana[1]; Colin Combe[2]; Lutz Fischer[3]; Marcus Bage[4]; Sameer Velankar[1]; Juri Rappsilber[2, 3]; Yasset Perez-Riverol[1]; Juan Antonio Vizcaíno[1]; *[1]EMBL-EBI, Hinxton, United Kingdom; [2]University of Edinburgh, School of Biological Sciences, Edinburgh, United Kingdom; [3]Technische Universität Berlin, Berlin, Germany; [4]EMBL-EBI, Hinxton, United Kingdom*

WP 400 **QCactus: interactive quality control software for statistical analysis and reporting metrics of raw proteomics data**; Zachary L Dwight[1]; Nathan Hendricks[1]; Santosh D Bhosale[1]; Jonathan T Bui[1]; Monica Ghaly[1]; Susan

M Mockus[1]; *[1]Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA*

WP 401 **KPOP: a standardized data repository for open access proteomics data**; Seungjin Na[1]; Hokeun Kim[2]; Jingi Bae[2]; Heeyoun Hwang[1]; Shinyeong Ju[3]; Cheolju Lee[3]; Jin Young Kim[1]; Sang-Won Lee[2]; Eunok Paek[4]; *[1]Korea Basic Science Institute, Cheongju, South Korea; [2]Korea University, Seoul, South Korea; [3]Korea Institute of Science and Technology, Seoul, South Korea; [4]Hanyang University, Seoul, South Korea*

WP 402 **Efficient Web Processing of Complex, Highly Dense LC/UV/MS Data Using High-Performance Computing Technologies**; Richard Lee[1]; Rostislav Pol[1]; Sofya Chudova[1]; *[1]ACD/Labs, Toronto, ON*

WP 403 **A downstream proteomics analysis and visualization platform with modular design, web-interface, and persistent storage**; Pierre Jean Beltran[1]; Liang Xue[1]; Robert V Stanton[1]; *[1]Pfizer, Inc, Cambridge, MA*

WP 404 **Hive: New File Format for Mass Spectrometry Measurement Data and Reader API**; Ipputa Tada[1]; Kazuto Mannen[1]; Mitsuhiro Kanazawa[1]; Atsushi Ogiwara[1]; *[1]Reifycs Inc., Tokyo, Japan*

WP 405 **A standardized workflow for extracting and storing MS1 isotope distribution information from LC-MS proteomics experiments**; Frédérique Vilenne[1]; Annelies Agten[1]; Dirk Valkenborg[1]; *[1]Hasselt University, Hasselt, Belgium*

WP 406 **QuaProt LIMS: a laboratory information management system for targeted proteomics assay development process**; Pallab Bhowmick[1]; Yassene Mohammed[1, 2, 3]; Christoph H. Borchers[1, 3, 4, 5]; *[1]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [2]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [3]Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; [4]Division of Experimental Medicine, McGill University, Montreal, QC; [5]Department of Pathology, McGill University, Montreal, QC*

WP 407 **New automation tool to remotely submit LC-MS data acquisition and processing for biopharmaceutical applications**; Stephane Houel[1]; Kevin Schauer[2]; Sega Ndiaye[3]; Jennifer Sutton[4]; Tara Schroeder[5]; Shannon Eliuk[6]; *[1]Thermo Fisher Scientific, Lexington, MA; [2]Thermo Fisher Scientific, Bannockburn, IL; [3]Thermo Fisher Scientific, Courtaboeuf, France; [4]ThermoFisher Scientific, San Jose, CA; [5]Thermo Fisher Scientific Inc, Somerset, New Jersey; [6]Thermo Fisher Scientific, San Jose, CA*

WP 408 **MSDMS: An Open Source Web Application to Design and Manage Custom Tandem Mass Spectrometry Libraries**; Quentin Rouchon[1, 2]; Gérard Hopfgartner[1]; *[1]LSMS, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; [2]Swiss Institute of Bioinformatics (SIB), Lausanne, Switzerland*

WP 409 **Cloud-based parallelization leads to a drastically faster library-free analysis in Spectronaut**; Grzegorz Skoraczyński[1]; Soham Garg[2]; Oliver M. Bernhardt[1]; Damiano Robbiani[1]; Amy Mann[2]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]Amazon Web Services, Seattle, WA*

WP 410 **An infinite well: harmonizing all public proteomics data for machine learning**; Siegfried Gessulat[1]; Vishal Sukumar[2]; Michael Graber[2]; Markus Schneider[2]; Alexander Hogrebe[1]; Samia Ben Fredj[2]; Lizi Mamisashvili[2]; Tobias Schmidt[2]; Daniel P Zolg[2]; Martin Frejno[2]; *[1]MSAID, Berlin, Germany; [2]MSAID, Garching, Germany*

WP 411 **MetaboLights - Open Access Metabolomics Resource**; Noemi Tejera[1]; Felix Xavier Amaladoss[1]; Callum Martin[1]; Thomas Payne[1]; Mark Williams[1]; Ozgur Yurekten[1]; Claire O'Donovan[1]; *[1]EMBL-EBI, Hinxton, United Kingdom*

WP 412 **MassIVE: enhancing public data accessibility through extensions to the Universal Spectrum Identifier standard**; Jeremy Carver[1, 2]; Nuno Bandeira[1, 2, 3, 4]; *[1]University of California San Diego, La Jolla, CA; [2]Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; [3]Department of Computer Science and Engineering, University of California San Diego, La Jolla, CA; [4]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

WP 413 **Enhanced usability in the MSstats family of statistical analysis software for quantitative mass spectrometry-based proteomics**; Devon Kohler[1]; Mateusz Staniak[2]; Deril Raju[1]; Sarah Szvetecz[1]; Anthony Wu[1]; Olga Vitek[1]; *[1]Northeastern University, Boston, MA; [2]University of Wrocław, Wrocław, Poland*

WP 414 **Efficient Processing of Large-Scale Data-Independent Acquisition Mass Spectrometry Proteomics Experiments Using Parallelized Cloud-Native Pipelines**; Andrew Nichols[1]; Seth Just[2]; Iman Mohtashemi[1]; Lee Cantrell[3]; Jian Wang[1]; Harendra Guturu[1]; János Kis[1]; Yuandan Lou[1]; Theodore Platt[1]; Serafim Batzoglou[1]; *[1]Seer, Inc., Redwood City, CA; [2]Seer, Inc, Redwood City, CA; [3]Seer Inc., Redwood City, CA*

WP 415 **PyC2MC: A novel software platform for the automated analysis of LC-HRMS data of complex mixtures**; Germain Salvato Vallverdu[1, 2]; Carlos Celis Cornejo[2, 3]; Martha L Chacon-Patino[2, 4]; Christopher Rüger[5]; Julien Maillard[2, 6]; Carlos Afonso[2, 7]; Christopher L Hendrickson[4]; Brice Bouyssiere[2, 3]; Pierre Giusti[2, 6]; Ryan P Rodgers[4, 8]; *[1]Université de Pau et des Pays de l'Adour, Pau Cedex 9, France; [2]International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Harfleur, France; [3]Université de Pau et des Pays de l'Adour, Pau, France; [4]National High Magnetic Field Laboratory, Tallahassee, Florida; [5]University of Rostock, Rostock, Germany; [6]TotalEnergies, Harfleur, France; [7]COBRA UMR 6014, Rouen, France; [8]International Joint Laboratory – iC2MC : Complex Matrices Molecular Characterization, Tallahassee, Florida*

WP 416 **Empower your proteomics research: streamline integration, automation, and analysis with MD 2.0 Dataset Service**; Anna Quaglieri[1]; Aaron Triantafyllidis[1]; Bradley Green[1]; Mark Condina[1, 2]; Paula Burton Ngov[1]; Giuseppe Infusini[1]; Andrew Webb[1, 3, 4]; *[1]Mass Dynamics, Melbourne, Australia; [2]University of South Australia, Adelaide, Australia; [3]WEHI, Parkville, Australia; [4]University of Melbourne, Parkville, Australia*

WP 417 **Significantly faster library-free dia-PASEF analysis with a Spectronaut integrated workflow in ProteoScape**; Grzegorz Skoraczynski[1]; Tejas Gandhi[1]; Oliver M Bernhardt[1]; Lukas Reiter[1]; Sven Brehmer[2]; Javier Lopez[2]; Heidi Vitrac[2]; Jose Abuin[2]; Tharan Srikumar[2]; Dennis Trede[3]; *[1]Biognosys, Zurich, Switzerland; [2]Bruker Daltonics Inc., Billerica, MA; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

WP 418 **A Comprehensive Analysis Pipeline for Phosphoproteomic Biomarker Discovery**; David N. Perkins[1]; Pedro Moreno-Cardoso[1]; Nazrath Nawaz[1]; Weronika E. Borek[1]; Josie A. Christopher[1]; Amy E. Campbell[1]; Andrew Williamson[1]; Arran D. Dokal[1]; *[1]Kinomica Ltd, Macclesfield, Cheshire, United Kingdom*

WP 419 **BioLadder: a bioinformatic platform primarily focused on proteomic data analysis**; Yupeng Zhang[1]; Lixin Wang[1]; Jinhao Wang[1]; Yunping Zhu[2]; Songfeng Wu[1]; Jingli Li[1]; *[1]Beijing Qinglian Biotech Co., Ltd,, Beijing, China; [2]State Key Laboratory of Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences (Beijing), Beijing Institute of Lifeomics, Beijing, China*

WP 420 **Streamlining PRM Method Development: A Novel Computational Interface**; Jaenyeon Kim[1]; Minsoo Son[1]; Young Ah Goo[1]; *[1]Mass Spectrometry Technology Access Center at McDonnell Genome Institute (MTAC@MGI) at Washington University School of Medicine, St. Louis, Missouri 64110*

WP 421 **Developing a regulatory compliant solution for nominal and accurate mass LC-MS spectrometry analysis in oligonucleotide therapeutics**; Kosuke Uchiyama[1]; Risa Suzuki[1]; Noriko Kato[1]; Yuka Fujito[1]; Neil J Loftus[2]; Simon

Ashton[2]; Stephane Moreau[3]; *[1]Shimadzu Corporation, Nakagyo-ku, Japan; [2]Shimadzu MS/BU, Manchester, United Kingdom; [3]Shimadzu Europa GmbH, Duisburg, Germany*

WP 422 **Thermal Proteome Profiling Analysis using FragPipe Platform**; Carolina Rojas Ramirez[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, Michigan*

WP 423 **The sky is the limit: a cloud-based proteomics platform for the masses**; Daniel P Zolg[1]; Markus Schneider[1]; Patroklos Samaras[1]; Samia Ben Fredj[1]; Florian Seefried[1]; Dulguun Bold[1]; Layla Eljagh[1]; Michelle Tamara Berger[1]; Alexander Hogrebe[1]; Siegfried Gessulat[1]; Tobias Schmidt[1]; Martin Frejno[1]; *[1]MSAID, Garching, Germany*

WP 424 **Longitudinal data quality monitoring enables improvement of quality management practices: a case study in proteomic research utilizing a digital-twin approach**; Tharan Srikumar[1]; Cassandra Wong[2]; Brendon Seale[2]; Torsten Michael Mueller[3]; Stefan Harsdorf[4]; Sergio Legaz[5]; Jonathan Krieger[1]; Dennis Trede[4]; Anne-Claude Gingras[2]; Matthew R Lewis[6]; *[1]Bruker Ltd., Milton, ON; [2]Lunenfeld-Tanenbaum Research Institute Mount Sinai Hospital, Toronto, Ontario; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [5]Bruker Daltonics GmbH & Co. KG, Billerica, MA; [6]Bruker UK Limited, Life Sciences Mass Spectrometry Division, Coventry, United Kingdom*

WP 425 **Streamlining Protein Complex Composition Analysis with an Integrated Informatics Workflow**; Daisha Utley[1]; Joseph B. Greer[1,2]; Kenneth R. Durbin[1]; Ryan T. Fellers[1,2]; Matthew T. Robey[1]; Neil L. Kelleher[1,2]; *[1]Proteinaceous, Inc., Evanston, IL; [2]Northwestern University, Evanston, IL*

WP 426 **ProteomicsDB: Connecting proteomes across species**; Armin Soleymaniniya[1,2]; Miriam Abele[3,4]; Sarah Brajkovic[2,4]; Christina Ludwig[2,3]; Bernhard Kuster[2,3,4]; Mathias Wilhelm[1,2]; *[1]Computational Mass Spectrometry, TUM, Freising, Germany; [2]Elite Network Bavaria, TUM, Freising, Germany; [3]Bavarian Center for Biomolecular Mass Spectrometry, TU Munich, TUM School of Life Sciences, Freising, Germany; [4]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany*

WP 427 **Integrated Data Analysis of Oligonucleotide Therapeutics Using LC-MS, LC-MS/MS and MALDI techniques**; Nishi Rochelle[1]; Neil J Loftus[2]; Simon Ashton[2]; Kosuke Uchiyama[3]; Risa Suzuki[3]; Takashi Nishikaze[3]; Yuka Fujito[3]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]Shimadzu MS/BU, Manchester, United Kingdom; [3]Shimadzu Corporation, Nakagyo-ku, Japan*

WP 428 **MiCId_GUI: The Graphical User Interface for MiCId, a Fast Microorganism Classification and Identification Workflow with Accurate Statistics and High Recall**; Aleksey Y Ogurtsov[1]; Gelio Alves[2]; Yi-Kuo Yu[2]; *[1]CBB NCBI NLM NIH, Bethesda, MD; [2]NIH, Bethesda, MD*

WP 429 **ASMS 2024 Abstract: Automated Analysis of Large-Scale Proteomics Datasets Using a Data-Analysis Platform, ProEPIC**; Ajay Bharadwaj[1]; Niveda Sundararaman[2,3]; Zachary Dwight[4]; Oliver Y Wang[2]; Rakhi Pandey[1]; Jennifer E. Van Eyk[1,3]; *[1]Cedars-Sinai Medical Center, Los Angeles, CA; [2]Cedars-Sinai Medical Center, Los Angeles; [3]Advanced Clinical BioSystems Research Institute, Cedars-Sinai Medical Center, Los Angeles, CA; [4]Cedars-Sinai Precision Biomarker Labs (PBL), Beverly Hills, CA*

WP 430 **Integration of Skyline and PDV into FragPipe for Advanced Visualization**; Fengchao Yu[1]; Matthew Chambers[2]; Kai Li[1]; Daniel Polasky[1]; Brendan MacLean[2]; Alexey Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, Michigan; [2]University of Washington, Seattle, WA*

WP 431 **A Common Data Analysis Pipeline (CDAP) for Data Independent Acquisition Mass Spectrometry Data**; Aaron Maurais[1]; Michael Riffle[1]; Brian Connoly[2]; Matthew Chambers[1]; Brendan X MacLean[3]; Gennifer E Merrihew[3]; Julia E Robbins[3]; Ratna R Thangudu[4]; Brian C. Searle[5]; Christine C Wu[3]; Paul A Rudnick[6]; Michael J. MacCoss[3]; *[1]University of Washington, Seattle, WA; [2]University of Washington - Laboratory Medicine and Pathology, Seattle, WA; [3]University of Washington - Genome Sciences, Seattle, WA; [4]ICF International, Reston, VA; [5]Ohio State University, Colubus, OH; [6]Spectragen Informatics, Bainbridge Island, WA*

WP 432 **New Outlier Detection Capabilities and Enhanced Reporting in Panorama and AutoQC**; Josh Eckels[1]; Ankur Juneja[1]; Wendy Innis[1]; Sweta Jewargikar[1]; Vagisha Sharma[2]; Nicholas Shulman[2]; Michael J. MacCoss[2]; Brendan MacLean[2]; *[1]LabKey, San Diego, CA; [2]University of Washington, Seattle, WA*

INSTRUMENTATION: MINI/PORTABLE/FIELDABLE MS
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WP 433 **A Gas Assisted Bi-helical Reconfigurable Ion Guide for Ambient Mass Spectrometry**; He Xingliang; *Sichuan University, Chengdu, China*

WP 434 **Portable Mass Spectrometer for Bioaerosol Detection**; Vadym Berkout[1]; Stuart Collymore[1]; Scott Ecelberger[1]; Max Cetta[1]; Lara Moore[1]; Michael McLoughlin[1]; Wayne Bryden[1]; *[1]Zeteo Tech, Inc., Sykesville, MD*

WP 435 **Development of a portable UPLC Mass Spectrometer**; Chung-Hsuan Chen[1]; Ju Yao Chang[1,2]; chun-jen Hsiao[1]; Jung Lee Lin[1]; *[1]Genomic Research Center, Taipei,, Taiwan; [2]National Sun Yat-Sen University, Kaohsiung, Taiwan*

WP 436 **Portable Instrumentation for SPME Analysis: Beyond the Laboratory**; Enrico Davoli[1]; Alessia Turina[1]; Stefano Carabellese[1]; Alice Passoni[1]; Vladimir M. Doroshenko[2]; *[1]Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy; [2]MassTech Inc., Columbia, MD*

WP 437 **Prototype Development of a Digital Linear Ion Trap based Palmtop Mass Spectrometer**; Saifei CHEN[1]; Yongkai CAI[1]; Lin LIU[1]; Hongbing CHENG[1]; Qiao JIN[1]; Yuanyuan HUANG[1]; Wenjian SUN[1]; *[1]Shimadzu Research Laboratory (Shanghai) Co.Ltd., Shanghai, China*

WP 438 **Pollinator Watch: Evaluating Environmental Contamination Through Beehive Air Volatiles with Portable Mass Spectrometric Systems**; Daria Ilić[1]; Boris Brkić[1]; Đorđe Vujić[1]; *[1]BioSense Institute, Novi Sad, Serbia*

WP 439 **Adapting a DART-MS seized drug analysis workflow to a field deployable, high-resolution mass spectrometry system**; Elizabeth L. Robinson[1]; Meghan G. Appley[1]; Thomas P. Forbes[1]; Edward Sisco[1]; *[1]NIST, Gaithersburg, MD*

WP 440 **An APPI Miniature Mass Spectrometer for Real-Time Analysis of BTEX**; David Lewis[1]; Kevin P Schultze[2]; Mac Gilliland[1]; *[1]Furman University, Greenville, SC; [2]908 Devices Inc., Boston, MA*

WP 441 **MOMA Engineering Test Unit Sample Investigation and Database Generation**; Friso H.w. Van Amerom[1,2]; Xiang Li[1]; Marco E Castillo[1,3]; Ryan M. Danell[1,4]; Desmond A. Kaplan[1,5]; Andrej Grubisic[1]; Teresa Fornaro[6]; William B Brinckerhoff[1]; And The MOMA Team[7]; *[1]NASA Goddard Space Flight Center, Greenbelt, MD; [2]Mini-Mass Consulting, Inc, Hyattsville, MD; [3]Aerodyne Industries, Cape Canaveral, FL; [4]Danell Consulting Inc, Winterville, NC; [5]KapScience LLC, Tewksbury, MA; [6]INAF-Astrophysical Observatory of Arcetri, Florence, Italy; [7]Max Planck Institut für Sonnensystemforschung, Goettingen, Germany*

WP 442 **Identification of Two Common Diagnostic Peptide Markers in Urine using a Portable Mass Spectrometer**; Dan Carmany[1]; Krisztian Torma[2]; William Yang Terziyan[2]; *[1]Self Employed, Las Vegas, NV; [2]BaySpec, Inc, San Jose, CA*

WP 443 **Performance of a planetary science instrument prototype with a dual source linear ion trap integrated to an Orbitrap analyzer**; Adrian Southard[1]; Lucas Taft Andrews[2]; Ryan M. Danell[3,4]; Desmond A. Kaplan[4,5]; Steven Rogacki[6]; Friso H.w. Van Amerom[4,7]; Ricardo Arevalo[2]; Niko Minasola[8]; Wally Rodriguez[8]; Diego Garcia[8]; *[1]CRESST-II Univ. of Maryland, CP, and NASA GSFC, Greenbelt, MD; [2]University of Maryland, College Park, College park, MD; [3]Danell Consulting, Inc., Winterville, NC; [4]NASA Goddard Space Flight Center, Greenbelt, MD; [5]KapScience LLC, Tewksbury, MA; [6]University of Michigan Space Physics*

Research Laboratory, Ann Arbor, MI; [7]Mini-Mass Consulting, Inc, Hyattsville, MD; [8]AMU Engineering Inc, Miami, FL

WP 444 **Simplified, abbreviated screening and confirmatory analysis of cocaine in urine matrix using BioSPME**; Caleigh R O'Connor[1]; Vladimir M. Doroshenko[1]; Enrico Davoli[2]; Nivedita Bhattacharya[3]; Jayeshkumar Das[1]; Venkat Panchagnula[1]; *[1]MassTech Inc., Columbia, MD; [2]Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy; [3]Barefeet Analytics Pvt. Ltd., Pune, India*

INSTRUMENTATION: NEW DEVELOPMENTS IN MASS ANALYZERS AND ION DETECTION

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WP 445 **Optimization of the Astral detection system: Enabling high linear dynamic range and single-ion sensitivity for deep proteome coverage**; Christian Hock[1]; Johannes Petzoldt[1]; Philipp Cochems[1]; Immo Colonius[1]; Bernd Hagedorn[1]; Arne Kreutzmann[1]; Daniel Mourad[1]; Maximilian Ochmann[1]; Amelia C. Peterson[1]; Hamish Stewart[1]; *[1]Thermo Fisher Scientific, Bremen, Germany*

WP 446 **A Novel Long-Lifetime Ion Detector for GC-TOFMS and GCxGC-TOFMS with Sub-Femtogram Detection Limits**; Matthew Soyk[1]; Semyon Shofman[2]; Amit Weingarten[2]; Viatcheslav Artaev[1]; *[1]LECO Corporation, St. Joseph, MI; [2]El Mul Technologies, Rehovot, Israel*

WP 447 **A novel long-life detector for a novel high-speed hybrid nominal mass platform**; Oleg Silivra[1]; Philip M. Remes[1]; Linfan Li[1]; Charles Maxey[1]; Cristina Jacob[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 448 **Multiple Ion Charge Extraction for High-Throughput Charge Detection Mass Spectrometry**; Raj Parikh[1]; Benjamin Draper[2]; Martin Jarrold[1]; *[1]Indiana University, Bloomington, IN; [2]Megadalton Solutions, Bloomington, Indiana*

WP 449 **A Digitally Operated Pre-filter Improves Transmission for Higher Stability Zones Accessed Using a Digital Quadrupole Mass Filter**; Fatima Olayemi Obe[1]; Elizabeth Groetsema[1]; Sumeet Chakravorty[1]; Gordon A Anderson[2]; Adam P. Huntley[1]; Brian H. Clowers[1]; Peter T. A. Reilly[1]; *[1]Washington State University, Pullman, WA; [2]GAA Custom Electronics LLC, Kennewick, WA*

WP 450 **Experimental Evaluation of the Higher Order Mathieu Space Stability Zones Using a Digitally Operated Mass Filter**; Sumeet S. Chakravorty[1]; Fatima O. Obe[1]; Elizabeth G. Groetsema[1]; Adam P. Huntley[1]; Gordon A. Anderson[2]; Brian H Clowers[1]; Peter T. A. Reilly[1]; *[1]Washington State University Department of Chemistry, Pullman, WA; [2]GAA Custom Electronics LLC, Kennewick, WA*

WP 451 **Characterization of RF Imbalance Influence on Black Holes in a Miniature Linear Ion Trap for Space Flight Applications**; Desmond A. Kaplan[1, 2]; Ryan M. Danell[1, 3]; Ryan Barnhart[4]; Jacob D. Graham[1]; Friso Van Amerom[1, 5]; Marco E. Castillo[1, 6]; William B. Brinckerhoff[1]; Andrej Grubisic[1]; Melissa G Trainer[1]; *[1]NASA Goddard Space Flight Center, Greenbelt, MD; [2]KapScience LLC, Tewksbury, MA; [3]Danell Consulting, Inc., Winterville, NC; [4]University of Michigan Space Physics Research Laboratory, Ann Arbor, MI; [5]Mini-Mass Consulting, Inc, Hyattsville, MD; [6]Aerodyne Industries LLC, Cape Canaveral, FL*

WP 452 **Development of a Digital Quadrupole Mass Filter with Improved Isolation Efficiency**; Robert Schrader[1]; Gordon A Anderson[2]; David H Russell[1]; *[1]Texas A&M University, College Station, TX; [2]GAA Custom Electronics LLC, Kennewick, WA*

WP 453 **Setting the STORI Straight: Improved CDMS Results Via misSTORI Analysis**; Michael Goodwin[1]; Kyle Patrick Bowen[1]; Dmitry Grinfeld[2]; Ping Yip[1]; Michael W Senko[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany*

WP 454 **Detecting High Energy Ions on a High Voltage LIT-MS with a Curved 45-degree Dynode**; Liam Dugan[1]; Mark E Bier[2]; *[1]Carnegie Mellon University, Pittsburgh, PA; [2]Carnegie Mellon University, Pittsburgh, Pennsylvania*

WP 455 **Extending the Linear Range of Capacitive Ultra-Wide-Range Current Amplifiers above Eleven Orders of Magnitude**; Cornelius Wendt[1]; Alexander Bohnhorst[1]; Simon Degen[1]; Ansgar T. Kirk[1]; *[1]ACKISION GmbH, Hannover, Germany*

WP 456 **Design and Performance Characterization of the Hardware and Electronics for Pulse Counting Detection with a Linear Ion Trap Mass Spectrometer**; Ryan M. Danell[1, 2]; Andrej Grubisic[1]; Jacob D. Graham[1]; Desmond A. Kaplan[1, 3]; Friso Van Amerom[1, 4]; Marco E. Castillo[1, 5]; David R. Durachka[1]; William B. Brinckerhoff[1]; Melissa G. Trainer[1]; *[1]NASA Goddard Space Flight Center, Greenbelt, MD; [2]Danell Consulting, Inc., Winterville, NC; [3]KapScience LLC, Tewksbury, MA; [4]Mini-Mass Consulting, Inc, Hyattsville, MD; [5]Aerodyne Industries LLC, Cape Canaveral, FL*

WP 457 **Characterisation of post translational modifications of proteins with ECD fragmentation on a trapped ion mobility spectrometry (TIMS) equipped FT-ICR**; C Logan Mackay[1]; Anthony J Devlin[1]; Anna Simmonds[1]; Christopher A Wootton[2]; Felicia Green[1]; *[1]Rosalind Franklin Institute, Harwell, United Kingdom; [2]Bruker Daltonik GmbH & Co. KG, Bremen, Germany*

WP 458 **Characterization of ScintiFast Scintillators in a Microchannel Plate based TOF Detector**; Joe Czekner[1]; Sasha Kadyshevitch[2]; Barak Lavi[2]; Stephen Ritzau[1]; Amit Weingarten[2]; *[1]Photonis Scientific, Sturbridge, MA; [2]El-Mul Technologies, Rehovot, Israel*

WP 459 **Practical Quadrupole Theory: Digital Quadrupoles vs. Traditional Sinusoidal Operation**; Randall E Pedder[1]; Luke Metzler[1]; Jacob Pasko[1]; Alex Miscovich[1]; Herb Gass[1]; Gordon Anderson[2]; *[1]Ardara Technologies, Ardara, PA; [2]GAA Custom Electronics LLC, Kennewick, WA*

WP 460 **Rapid and Reliable Nitrite Content Analysis in Pharmaceutical Excipients with the ACQUITYTM QDaTM II Mass Detector**; Henry Foddy[1]; Amy Bartlett[1]; Victoria Starkie[1]; Jonathan Pugh[1]; Cristian Cojocariu[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

ION MOBILITY: FAIMS/DMS

461-467

WP 461 **Exploring bacterial virulence factors diversity using Field Asymmetric Ion Mobility Spectrometry (FAIMS) and Kendrick Mass Defect (KMD) Plots**; Abanoub Mikhael[1, 2]; Darryl Hardie[1]; Helena Pětrošová[1, 2]; ROBERT K ERNST[3]; DAVID R GOODLETT[1, 2]; *[1]UVic Genome BC Proteomics Centre, Victoria, BC; [2]University of Victoria, Victoria, BC; [3]University of Maryland, Baltimore, Baltimore, MD*

WP 462 **Novel Protein Separations Employing the Second Derivative of High-Field Ion Mobility in a Field Gradient**; Atena Tajaddodi[1]; Hayden A Thurman[1]; Alexandre A Shvartsburg[1]; *[1]Wichita State University, Wichita, KS*

WP 463 **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[1]; Luc A. Tessier[1]; Tammy-Lynn Tremblay[1]; Tyler M. Renner[1]; Jennifer J. Hill[1]; *[1]National Research Council of Canada, Ottawa, ON*

WP 464 **Optimization of LC-FAIMS-MS/MS for in-depth proteome characterization of plasma from cattle**; Gustavo Diaz[1]; Dorathea Lee[1]; Corey D Broeckling[1]; *[1]Analytical Resources Core: Bioanalysis and Omics Center, Colorado State University, Fort Collins, CO*

WP 465 **A Sensitive Antibody-free FAIMS-dCV/SRM-MS Method for Targeted Protein Quantification**; Qingqing Shen[1]; Jie Pu[1]; Chao Xue[1]; Ming Zhang[1]; Shihan Huo[1]; Wei-Jun Qian[2]; Cornelia L Boeser[3]; Michael W Belford[3]; Charles Maxey[3]; Neloni R. Wijeratne[3]; Claudia Martins[3]; Scott M Peterman[3]; Wang Cao[4]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]Pacific Northwest National Laboratory, Richland, WA; [3]ThermoFisher Scientific, San Jose, CA; [4]University at buffalo, buffalo*

WP 466 **Evaluation of FAIMS Coupled with the Orbitrap Astral Mass Spectrometer for Proteomics**; Li-Yu Chen[1];

Katherine A Overmyer[2, 3, 4]; Pavel Sinitcyn[3]; Scott T Quarmby[2]; Joshua J Coon[1, 2, 3, 4]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Morgridge Institute for Research, Madison, WI; [4]National Center for Quantitative Biology of Complex Systems, Madison, WI*

WP 467 **Assessing the reduction of interferences in SWATH data-independent acquisition (DIA) with differential mobility separation (DMS)**; Yves Le Blanc[1]; Eva Duchoslav[2]; Lyle Burton[2]; Bradley Schneider[2]; *[1]SCIEX, Concord, On, ON; [2]SCIEX, Concord, ON*

ION MOBILITY: GENERAL
468-481

WP 468 **Investigation the Effect of Travelling Wave Profiles in Structure for Lossless Ion Manipulation (SLIM)**; Mohsen Latif[1]; Viraj Gandhi[1, 2]; Leyan Hua[1]; Carlos larriba-andaluz[1]; *[1]Mechanical Engineering, IUPUI, Indianapolis, IN; [2]Purdue University, West Lafayette, IN*

WP 469 **IonToolPack: a software suit of AI-powered tools for mass spectrometry**; Aivett Bilbao[1]; Andrea Harrison[1]; Samiha Chabane[1]; Ashfiqur Rahman[1]; Nathalie Munoz[1]; Yuqian Gao[2]; Marija Velickovic[1]; Josie G. Eder[2]; Priscila Lalli[2]; Daniel J. Orton[2]; Chaevien S. Clendinen[1]; Vimal K. Balasubramanian[1]; Arunima Bhattacharjee[1]; Christopher R. Anderton[1]; Sarah M. Williams[1]; Sneha P. Couvillion[2]; Thomas L. Fillmore[1]; Karl K. Weitz[2]; Joonhoon Kim[3]; Young-Mo Kim[2]; Tao Liu[2]; Jennifer E. Kyle[2]; Kyle R. Pomraning[3]; Kristin E. Burnum-Johnson[1]; *[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; [2]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [3]Energy Processes and Materials Division, Pacific Northwest National Laboratory, Richland, WA*

WP 470 **Dual-Path TW-SLIM for Masked Ion Mobility Spectrometry with Complete Ion Utilization**; Cullen Greer[1]; Brian H Clowers[1]; *[1]Washington State University Department of Chemistry, Pullman, WA*

WP 471 **Lowering the Entry Barrier: A Low-Cost Vacuum Enclosure for Ion Funnels, Ion Guides, and Structures for Lossless Ion Manipulations**; Brian H. Clowers[1]; Nathan W. Buzitis[1]; Gustavo Gallardo[1]; *[1]Washington State University, Pullman, WA*

WP 472 **High-efficiency electron capture dissociation of peptides and proteins after collision-induced unfolding and ion mobility**; Joseph C. Meeuwsen[1]; Ruwan T. Kurulugama[1]; Yury V. Vasilev[1]; Valery G. Voinov[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 473 **Comparison of LC-MS/MS, LC-TIMS-MS/MS, and MALDI TIMS MS/MS Methods for Lipidomics**; Min Liu[1]; Carolina Cruz Cepeda[1]; John M. Koomen[1]; *[1]Moffitt Cancer Center, Tampa, FL*

WP 474 **Trends in Transition Metal Binding with Polyproline Using Ion Mobility Mass Spectrometry**; Anthony J Pestritto[1]; David Clemmer[1]; *[1]Indiana University, Bloomington, IN*

WP 475 **Sub-Nyquist Experimental Timescales Using Compressed Sensing Ion Mobility Mass Spectrometry**; Elvin R. Cabrera[1]; Brian H. Clowers[1]; *[1]Washington State University Department of Chemistry, Pullman, WA*

WP 476 **Utilizing High Resolution Ion Mobility Spectrometry-Mass Spectrometry for Opioid Profiling**; Jack P. Ryan[1]; James N. Dodds[1]; Erin S. Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

WP 477 **Cross Platform Assessment of Feature Detection Capability as a Function of Measured Resolving Power in Ion Mobility Spectrometry (IMS)**; James Dodds[1]; Amie M. Solosky[1]; Jack P. Ryan[1]; Erin S. Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

WP 478 **Moving IMS to the next level, New Possibilities with Multilevel SLIM**; Adam P. Huntley[1]; Adam L. Hollerbach[1]; Randolph V. Norheim[1]; Ahmed M. Hamid[1]; Gordon A Anderson[2]; Sandilya V.B. Garimella[1]; Jon M. Jacobs[1]; Richard D. Smith[1]; Yehia M Ibrahim[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]GAA Custom Electronics LLC, Kennewick, WA*

WP 479 **Accurate CCS Measurement by Multi-pass Cyclic IMS Enables Confident Glycan Structure Assignment**; Chaoshuang Xia[1]; Elias Mernie[1]; Joseph Zaia[1]; Catherine E. Costello[1]; Cheng Lin[2]; *[1]Boston University Chobanian & Avedisian School of Medicine, Boston, MA; [2]Boston University, Boston, MA*

WP 480 **Dendrimers and their application as mass and mobility calibration standards – a case study for reliability and applicability**; Jens Sommertune[1]; Emily R. Sekera[2, 3]; Claudia Möckel[4]; Florian Stappert[5]; Cedric Thom[5]; Arpad Somogyi[3]; Bela Paizs[6]; Oliver J Schmitz[5]; *[1]Polymer Factory Sweden, Stockholm, Sweden; [2]St Jude Children's Research Hospital, Memphis, TN; [3]Ohio State University, Columbus, OH; [4]Stockholm University, Stockholm, Sweden; [5]University of Duisburg-Essen, Essen, Germany; [6]Rosalind Franklin Institute, Didcot, United Kingdom*

WP 481 **Solving the "General Elution Problem" in Ion Mobility Spectrometry**; Eric Davis[1]; Tristan Koop[1]; Landon Vyhmeister[1]; Saned Gharari[1]; Julia Fehr[1]; Gavin Valdez[1]; *[1]Whitworth University, Spokane, WA*

LC/MS: CHROMATOGRAPHY AND SOFTWARE
482-494

WP 482 **Accurate mass spectral deconvolution of multiply-charged oligonucleotides using unit resolution single quadrupole LC/MS**; Patrick M Batoon[1]; Lee Bertram[2]; Yongdong Wang[3]; *[1]Agilent Technologies Inc., Santa Clara, CA; [2]Agilent Technologies, Santa Clara, CA; [3]Cerno Biosciences, Las Vegas, NV*

WP 483 **Rapid QC-MS – Interactive Dashboard for Near Synchronous Mass Spectrometry Data Acquisition Quality Control**; Wasim Sandhu[1]; Ira J. Gray[1]; Sarah Lin[1]; Joshua E. Elias[1]; Brian C. DeFelice[1]; *[1]Chan Zuckerberg Biohub, San Francisco, CA*

WP 484 **Evaluation of analytical columns in ADC separation for calculation of drug-to-antibody ratio (DAR)**; Kazuko Inoue; *Eisai Co.,Ltd., Tsukuba, Japan*

WP 485 **Automated Online LC-MS Small Molecule Reaction Monitoring with a Single Quadrupole MS**; Dr. Sebastian T. Weinig-Berger[1]; Russell Burge, PhD[2]; Dr. Edgar Naegele[1]; Dr. Andreas Mielcarek[1]; *[1]Agilent Technologies, Waldbronn, Germany; [2]Agilent Technologies Inc., Santa Clara, CA*

WP 486 **A Rational Strategy of Peptide Solubilization for Bottom-up Proteomics Using Hydrophilic Interaction Chromatography**; Eisuke Kanao[1, 2]; Koshin Akamatsu[1]; Ayana Tomioka[1]; Yasushi Ishihama[1, 2]; *[1]Kyoto university, Kyoto, Japan; [2]National Institutes of Biomedical Innovation, Health and Nutrition, Ibraki, Japan*

WP 487 **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 488 **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[1]; Kazutaka Ikeda[1]; *[1]Kazusa DNA Research Institute, 2-6-7 Kazusakamatari, Kisarazu, Japan*

WP 489 **Versatile use of microfluidic LC columns, optimized configuration for achieving significant increases in proteome coverage at low nanoLC flow rates**; Jeff Op De Beeck[1]; Natalie Van Landuyt[1]; Robert Van Ling[2]; Yuan Lin[3]; Paul Jacobs[1]; *[1]Thermo Fisher Scientific, Ghent, Belgium; [2]Thermo Fisher Scientific - Breda, Breda, Netherlands; [3]Thermo Fisher Scientific, Sunnyvale, CA*

WP 490 **Enhanced lipidomics analysis with phenyl-hexyl based RPLC-MS**; Yikun Liu[1]; Jinling Lu[1]; Wenpeng Zhang[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China*

WP 491 **Vendor-neutral, Browser-Based Advanced MS Data Processing**; Ryan Andrews[1]; Anne Marie Smith[1]; Richard

Lee[1]; Sofya Chudova[1]; Vitaly Lashin[1]; Rostislav Pol[1]; *[1]ACD/Labs, Toronto, ON*

WP 492 **Method Development of PFAS Compounds Using a Virtual Method Development Tool**; Melinda D Urich[1]; Justin Steimling[1]; Chris Nelson[1]; Tim Yosca[1]; John Garrett[2]; Elena Gairloch[1]; *[1]Restek Corporation, Bellefonte, PA; [2]Analytical Innovations, Dayton, OH*

WP 493 **Elevating Precision in Single-Cell Applications: A Breakthrough with Monolithic Silica Capillary Columns**; Michael Krawitzky[1, 2]; Mario Mirabelli[2]; Florian Busch[2]; Goran Mitulovic[2]; Jean-François Greisch[2]; Gary Kruppa[3]; *[1]Bruker Daltonics, San Jose, CA; [2]Bruker Switzerland AG, Faellanden, Switzerland; [3]Bruker S.R.O., Brno, Czech Republic*

WP 494 **On-line HIC-MS for the Analysis of ADCs**; Steven C Pomerantz[1]; Eilyn Lacy[1]; Richard Huang[1]; Steven Jacobs[1]; *[1]Janssen Research and Development, Spring House, PA*

LC/MS: SAMPLE PREPARATION II
495-514

WP 495 **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 496 **Development of a Portable and Rapid Hydrogel-Based Proteomic Workflow**; Maor Arad[1, 2]; Connor Frey[1, 2]; Rhien Hare[2, 3]; Ronald Balagtas[2]; Dario Jereb[2]; Zach Nestman[2]; Manjot Benning[2]; Kenneth Ku[2]; Osei Fordwour[1]; Golfam Ghafourifar[2]; Leonard J Foster[1]; *[1]University of British Columbia, Vancouver, BC; [2]University of the Fraser Valley, Abbotsford, BC; [3]Simon Fraser University, Burnaby, BC*

WP 497 **Sample Preparation and Cleanup of Adeno-Associated Virus 6 (AAV6) Capsid Proteins for LC-MS Characterization**; Sitora Khodjaniyazova[1]; Thomas Raymond Slaney[1]; *[1]Bristol Myers Squibb, New Brunswick, NJ*

WP 498 **Quantitative Analysis of Legacy & Emerging PFAS in Semiconductor Lubricant using Triple Quadrupole LC/MS**; Stephan Baumann[1]; Aimei Zou[2]; *[1]Agilent Technologies Inc., Atlanta, GA; [2]Agilent Technologies Singapore, Singapore, Singapore*

WP 499 **Development and optimization of a method for automated peptide desalting on the DigestPro MSi robot using AttractSPE® C18 tips**; Célia Jardin[1]; Soumia Hamada[1]; Cédric Pionneau[1]; Martin Technau[2]; Mana Shafaei[3]; Florine Hallez[4]; Michel Arotçarena[4]; Sami Bayoudh[4]; Kaynoush Naraghi[4]; Solenne Chardonnet[1]; *[1]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; [2]CEM GmbH, Kamp-Lintfort, Germany; [3]AFFINISEP USA, Miami, FL; [4]AFFINISEP, Le Houlme, France*

WP 500 **Fast and Efficient LC-MS/MS Analysis of PFAS for Clinical Research Using Microelution SPE**; Shahana Wahab Huq[1]; Galo Orquera-Aguirre[1]; Stephanie J. Marin[1]; *[1]Phenomenex, Torrance, CA*

WP 501 **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 502 **Proteonano™: a nanobinder-based deep proteomics platform for complex biofluid sample analysis enabling detection of a wide dynamic range of proteins**; Ziquan Cao[1]; Xiehua Ouyang[1]; Libing Wang[1]; Shanshan Lv[1]; Xin Du[1]; Yanting Meng[1]; Yonghao Zhang[1]; Yi Wang[1]; Jie Jin[2, 3]; Yang Li[2, 3]; Hao Wu[1]; *[1]Nanomics Biotechnology, Hangzhou, China; [2]Wuhan Biorun BioSciences Co.,Ltd, Wuhan, China; [3]Wuhan Institute of Biotechnology, Wuhan, China*

WP 503 **High-throughput and automated cellular and tissue lysis using COVARIS acoustic technology for proteomics**; Josselin Ortiz[1]; Angel Keoseyan[1]; Santosh D Bhosale[1]; Nathan Hendricks[1]; Saeed Seyedmohammad[2]; Sameer Vasantgadkar[3]; Lia Abarzua[3]; Annie Moradian[1]; Susan M. Mockus[1]; Jennifer E. Van Eyk[1, 2]; *[1]Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA; [2]Smidth Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA; [3]Covaris, LLC, Woburn, MA*

WP 504 **Characterization of the New PAL Micro-SPE Cartridge for Pesticides Extract Clean-up**; Jonathan Beck[1]; Hans-Joachim Huebschmann[2]; Lucas Luethy[2]; *[1]CTC Analytics AG, Lake Elmo, MN; [2]CTC Analytics AG, Zwingen, Switzerland*

WP 505 **Automated workflow for antibody production and analysis on a robotic liquid handling platform**; Boren Lin[1]; Rinat R Abzalimov[2]; Kinnari Watson[1]; *[1]Opentrons Labworks, New York, NY; [2]Advanced Science Research Center, The City University of New York, New York, New York*

WP 506 **Investigating Greener Alternative Detergents for Application in MS Sample Preparation**; Joanna M Gongora[1]; Francisca N De Luna Vitorino[1]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

WP 507 **Analysis of 6PPD-Quinone in Salmon: A Simplified Sample Prep**; Tina Chambers[1]; Jennifer Cottine Hitchcock[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 508 **Bioanalytical quantification of a lipid conjugated anti-sense oligonucleotide on a HRMS system**; Nikunj Tanna[1]; Mary Trudeau[1]; Joe Fredette[1]; *[1]Waters Corporation, Milford, MA*

WP 509 **Improved Tissue Homogenization and SPE-Based Sample Preparations for the Quantitative LC-MS analysis of Oligonucleotide Therapeutics**; Makda Araya[1]; Kim Tran[1]; Mary Trudeau[1]; Joe Fredette[1]; Bala Addepalli[1]; Matthew Lauber[1]; *[1]Waters Corporation, Milford, MA*

WP 510 **Formulation-specific consumer products analysis for alleviating ion-suppression in MS**; Hyeonjeon Cha[1]; Tae-Young Kim[1]; *[1]School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea*

WP 511 **A new Approach to Optimising the SPE Extraction of Oligonucleotides**; Colin Pipe[1]; David Dunthorne[1]; Tony Edge[1]; Matthew James[1]; Ed Faden[2]; *[1]Avantor, Theale, United Kingdom; [2]MAC-MOD, Chadds Ford, PA*

WP 512 **An improved EasyPep sample preparation method for enrichment and quantitation of host cell proteins**; Jae Choi[1]; Cristina C Jacob[2]; Philip Remes[2]; Oleg Silivra[2]; Terry Hicks[3]; Matthew Daniels[3]; Nikki Jarrett[1]; Kay Opperman[1]; Bhavin Patel[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, St. Louis, MO*

WP 513 **Mitigating Cross-Contamination of Methamphetamine in Urine During Supported Liquid Extraction**; Alicia Robinson[1]; Yuping Wang[1]; Lamvien Nguyen[1]; James LaPalme[1]; Elizabeth Bair[1]; Ona Adair[1]; *[1]SC PHL, Columbia, SC*

WP 514 **High-pH reversed-phase peptide fractionation on innovative SPE microelution well plates for high-throughput and automated workflows in proteomic studies**; Kaynoush Naraghi[1]; Mana Shafaei[2]; Florine Hallez[1]; Michel Arotçarena[1]; Sami Bayoudh[1]; Cerina Chuuon[3]; Chiara Guerrera[3]; *[1]AFFINISEP, Le Houlme, France; [2]AFFINISEP USA, Miami, FL; [3]INSERM – US24 SFR Necker Proteome, Paris, France*

METABOLOMICS: TARGETED AND QUANTITATIVE ANALYSIS I
515-535

WP 515 **High Throughput Targeted Metabolomics Library Generation on a Novel Mass Spectrometer Applied to Microbiome Analysis**; Bashar Amer[1]; Cristina Jacob[1]; Rahul Deshpande[1]; Reza Jafari[2]; Thomas Moehring[3]; Susan S Bird[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]MetaSci, Toronto, Ontario; [3]Thermo Fisher Scientific, Bremen, Germany*

WP 516 **A combined targeted-untargeted metabolomics workflow for the identification and quantitation of metabolites in complex matrices**; Paul RS Baker[1]; Rebekah Sayers[2]; Cagakan Ozbalci[2]; Robert Proos[1];

[1]*SCIEX, USA, Framingham, MASSACHUSETTS;* [2]*SCIEX UK, Macclesfield, United Kingdom*

WP 517 **An improvised method for simplified simultaneous quantitation of the constituents of a chemically complex mixture**; Chris Beecher[1]; Vladimir Shulaev[2]; Debasish Ghosh[2]; Felice de Jong[1]; Alexander Raskind[1]; [1]*IROA Technologies LLC, Nellysford, VA;* [2]*UNIVERSITY OF NORTH TEXAS, Denton, TX*

WP 518 **Widely targeted volatilomics and volatile-GWAS based aromatic rice breeding**; Jie Luo; *Hainan University, Sanya, China*

WP 519 **Quantification of TCA cycle metabolites with automated sample prep, reproducible HILIC chromatography and ion funnel triple quadrupole**; Bianca Ferreira da Silva[1]; Cate Simmermaker[2]; Sierra D. Durham[2]; Karen E. Yannell[2]; [1]*Agilent Technologies, Lexington, MA;* [2]*Agilent Technologies, Santa Clara, CA*

WP 520 **Metabolomic Characterization of a Perfusion Bioprocess System using Pyxis – A Machine Learning Tool for Absolute Quantitation**; Erin Weisenhorn[1]; Luke S. Ferro[2]; Jack Howland[2]; Jonathan Mene[1]; Rosemichelle Marzan[1]; Matthew Stebbins[1]; Eric Rynes[1]; Timothy Kassis[2]; Ana S.H. Costa[2]; Jefferson G. Pruyne[2]; Devesh Shah[2]; Joshua D. Lauterbach[2]; Tian Cai[2]; Jennifer M Campbell[2]; Geoffrey Horner[1]; [1]*Just - Evotec Biologics, Seattle, WA;* [2]*Matterworks, Somerville, MA*

WP 521 **Comprehensive analysis of the NAD+ metabolome in human serum**; Helena Li[1, 2]; Junfang Zhao[2]; Siara Michels[1, 2]; Kenneth D.R. Setchell[2]; Lindsey Romick[2]; Xueheng Zhao[2]; [1]*University of Cincinnati, Cincinnati, OH;* [2]*Division of Pathology & Laboratory Medicine, Cincinnati Children's Hospital Medical Center, Cincinnati, OH*

WP 522 **Correlation of soluble metabolites with Lactate Switch Observed in HEK293 Culture using Novel CE-MS Metabolomics Workflow**; Catherine Rawlins[1]; Erin Redman[2]; Milla Neffling[1]; Stephanie Klaubert[1]; Awab Nehala[1]; J. Will Thompson[2]; [1]*908 Devices Inc., Boston, MA;* [2]*908 Devices Inc., Morrisville, NC*

WP 523 **MASS SPECTROMETRY BASED NUTRIMETABAlOMICS AS A POWERFUL PLATFORM FOR MILLETS**; Sugasini Dhavamani[1]; Anchal Sharma[2]; Prasanth Kumar Punathil Kannan[3]; Raja Lakshitha[4]; Vidya Gundlapalli[5]; Nicole Lysik[6]; Sutape Chantapim[6, 7]; [1]*Department of Medicine,University of Illinois at Chicago, Chicago, IL;* [2]*Department of Chemistry, Research Core Facility, University of Illinois at Chicago, Chicago, IL;* [3]*Department of Pediatrics, University of Illinois at Chicago, Chicago, IL;* [4]*Tamilnadu Agricultural University, Madurai, India;* [5]*Department of Chemistry, Loyola University, Chicago, IL;* [6]*Department of Medicine, University of Illinois Chicago, Chicago, IL;* [7]*University of Illinois at Chicago, Chicago, IL*

WP 524 **NADomic LCMS separating isobaric and close-mass metabolites in both salvage and kynurenine pathways**; Rong Meng[1]; Katharine D'Aquino[1]; Jose Antonio Chavez[1, 2]; Annette Eckardt[1]; Tobias Schips[1]; Karl Kavalkovich[1]; Simon Hinke[1]; Andrea Nawrocki[1]; [1]*Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania;* [2]*Quotient Therapeutics, Cambridge, MASSACHUSETTS*

WP 525 **Simultaneous consideration of within-injection and cross-injection aggregated EIC properties for improved quantitation in LC-MS MRM metabolomics datasets**; Phillip Seitzer[1]; Alireza Delfarah[1]; Johanna Fleischman[1]; Edward S Folk[1]; Celeste Sandoval[1]; Ngoc Vu[1]; Bryson Bennett[1]; [1]*Calico Life Sciences, LLC, South San Francisco, CA*

WP 526 **A high-sensitivity UPLC-MRM/MS method for metabolomic analysis of isoprenoid lipids**; Jun Han[1, 2]; Juncong Yang[1]; Katelyn McMurray[1]; Malia Lampard[1]; Dave Schibli[1, 2]; David R Goodlett[1, 3]; [1]*Genome BC Proteomics Centre, University of Victoria, Victoria, BC;* [2]*Division of Medical Sciences, University of Victoria, Vicotria, BC;* [3]*Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC*

WP 527 **Validation of Targeted Quantitative Analysis of Endogenous Biomarkers for Good Clinical Practice Studies**; Maggie Rossow[1]; Lisa Ford[1]; Deirdre Hauser[1]; Anne M Evans[1]; [1]*Metabolon Inc., Morrisville, NC*

WP 528 **A novel ML approach to rapidly analyze changes in metabolite concentrations in algae fermentation for bioprocess optimization**; Jack Howland[1]; Frank Xu[2]; Bokkyoo Jun[2]; Yao Lu[2]; Lisa Laprade[2]; Travis Korosh[2]; Luke S Ferro[1]; Ana S.H. Costa[1]; Joshua D. Lauterbach[1]; Jefferson G. Pruyne[1]; Devesh Shah[1]; Timothy Kassis[1]; Jennifer M Campbell[1]; [1]*Matterworks, Inc., Somerville, MA;* [2]*DSM North America, Columbia, MD*

WP 529 **Evaluating a Novel Microchip CE Platform for Use in High-Throughput Quantitative Metabolomics**; Cristina Di Poto[1]; Xiang Tian[1]; Hampus Engstroem[2]; Erin A. Redman[2]; J. Scott Mellors[2]; J. Will Thompson[2]; Sonja Hess[1]; Erik L. Allman[1]; [1]*Dynamic Omics, Centre for Genomics Research (CGR), Discovery Sciences, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD;* [2]*908 Devices Inc., Morrisville, NC*

WP 530 **Targeted Desorption Electrospray Ionization Mass Spectrometry Imaging For Central Carbon Metabolite Distribution In Mouse Tissue Samples**; Virag Sagi-Kiss[1]; Yayue Song[2]; Brittannie Willis[1, 2]; Daniel Simon[1, 3]; Duncan Connor Roberts[1]; Suqian Zhang[2]; Simone Di Giovanni[2]; Harry J Whitwell[1]; Zoltan Takats[1]; [1]*Department of Metabolism, Digestion and Reproduction; Imperial College London, London, United Kingdom;* [2]*Division of Neuroscience, Department of Bain Sciences, Imperial College London, London, United Kingdom;* [3]*Rosalind Franklin Institute, Harwell, United Kingdom*

WP 531 **Disrupted Lipid Metabolism and Cardiomyopathy: Unraveling the Impact of Mitochondrial Fission Factor Loss through Multi-Organ Targeted Metabolomics**; Prasanna Vadhana Ashok Kumaar[1]; Olga Bielska[1]; Wendy Jara[1]; Anne Marker[1]; Birgit Schilling[1]; Eric Verdin[1]; [1]*Buck Institute for Research on Aging, Novato, CA*

WP 532 **From structure to signal: prediction of molecular response rates in mass spectrometry from 3D conformations**; Yuhui Hong[1]; Chhavi Thakur[1]; Sujun Li[1, 2]; Christopher J Welch[3]; Haixu Tang[1]; [1]*Indiana University Bloomington, Bloomington, IN;* [2]*GlycoMS LLC, Bloomington, IN;* [3]*Indiana Consortium for Analytical Science & Engineering (ICASE), Indianapolis, IN*

WP 533 **Targeted Metabolic Profiling of Tryptophan, Tyrosine and Branched Chain Amino Acid Metabolism**; Vladimir Shulaev[1]; Debasish Ghosh[1]; Geoff Faden[2]; Ed Faden[2]; [1]*University of North Texas, Denton, TX;* [2]*MAC-MOD Analytical, Chadds Ford, PA*

WP 534 **Influence of sex and high-fat diet on the regional heterogeneity of bile acid profiles in the intestine of C57BL/6 mice**; Yan Ni[1]; Chuanhao Yang[1, 2]; Ana Liu[1]; Huiying Wang[1]; Hongtao Liu[1, 2]; Cuifang Xu[1]; Rong Rong[2]; Qingtao Lv[2]; [1]*Children's Hospital, Zhejiang University School of Medicine, National Clinical Research Center for Child Health, Hangzhou, China;* [2]*Shandong University of Traditional Chinese Medicine, Jinan, China*

WP 535 **Method development for quantitatively measuring sex steroids in plasma or serum**; Linxing Yao[1]; Corey Broeckling[1]; [1]*Colorado State University, Fort Collins, CO*

NEUROSCIENCE AND NEURODEGENERATIVE DISEASE RESEARCH II
536-560

WP 536 **Multimodal analysis of neurodegeneration related changes in lipidomic profiles as a function of diet**; Catelynn C Shafer[1]; Jacopo Di Lucente[1]; Izumi Maezawa[1]; Lee-Way Jin[1]; Elizabeth K Neumann[1]; [1]*UC Davis, Davis, CA*

WP 537 **Characterization of brain α-synuclein in neurodegenerative diseases by high-resolution mass spectrometry**; Kim-Thanh VAN[1]; Nicolas Villain[2]; Foudil Lamari[2]; Susana Casas BOLUDA[2]; François Fenaille[1]; François Becher[1]; [1]*CEA Paris-Saclay, Gif sur Yvette,* *France; [2]Hôpitaux Universitaires Pitié Salpêtrière, Paris, France*

WP 538 **A silicon nanodialysis probe coupled with ZipChip CE-MS enables localized in vivo sampling for monitoring brain chemistry**; Keyin Li[1]; Weihua Shi[1]; Yu Ding[1]; Alex George Armstrong[1]; Stanislav Rubakhin[1]; Yurii A Vlasov[1]; Jonathan V Sweedler[1]; *[1]university of Illinois-Urbana Champaign, Urbana, IL*

WP 539 **In-depth proteome profiling of the hippocampus of Ldlr knockout mice reveals alternation in the synaptic signaling pathway**; Hong-Beom Park[1, 2, 3]; Hosek Seo[2, 3, 4]; Eunji Jeon[2, 3]; Gyuri Park[3, 5]; Hyeon Chang Lee[3, 5]; Jayun Choi[3, 6]; Sinae Lee[3, 6]; Dohyun Han[2, 3]; *[1]Department of Biomedical Science, College of Medicine, Seoul National University, Seoul, South Korea; [2]Department of transdisciplinary medicine, Seoul National University Hospital, Seoul, South Korea; [3]Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; [4]Interdisciplinary Program in Neuroscience, College of Natural Sciences, Seoul National University, Seoul, South Korea; [5]Molecular Medicine and Biopharmaceutical Sciences, WCU Graduate School of Convergence Science and Technology Seoul National University, Seoul, South Korea; [6]Cancer Research institute, Seoul National University college of medicine, Seoul, South Korea*

WP 540 **Multi-omics Evaluation of Human iPSCs and iPSC-derived Neurons**; Gwangbin Lee[1]; Wan Nur Atiqah Binti Mazli[1]; Ling Hao[1]; *[1]Department of Chemistry, George Washington University, Washington, DC, United States, Washington, D.C., DC*

WP 541 **CEREBROSPINAL FLUID APOE GLYCOSYLATION ASSOCIATES WITH BIOMARKERS OF ALZHEIMER'S DISEASE PATHOLOGY**; Dobrin Nedelkov[1]; Zoe Tsokolas[2]; Isabel Sible[2]; Wendy J Mack[2]; S Duke Han[2]; John SC Rodman[2]; Hussein N Yassine[2]; *[1]Isoformix, Sugar Land, TX; [2]University of Southern California, Los Angeles, CA*

WP 542 **Proteomic analysis on Postmortem Brain Tissue for Molecular Characterization of Chronic Neurodegenerative Diseases Induced by Traumatic Brain Injury**; Junho Park[1, 2]; Dongyoon Shin[2]; Dohyun Han[3, 4]; Yeongshin Kim[5]; Hoon Ryu[6, 7, 8]; Youngsoo Kim[2, 5]; *[1]Department of Pharmacology, CHA University School of Medicine, Seongnam-si, South Korea; [2]Proteomics Research Team, CHA Future Medicine Research Institute, Seongnam-si, South Korea; [3]Proteomics Core Facility, Biomedical Research Institute, Seoul, South Korea; [4]Transdisciplinary Department of Medicine & Advanced Technology, Seoul National University Hospital, Seoul, South Korea; [5]Department of Medical Science, CHA University School of Medicine, Seongnam-si, South Korea; [6]Boston University Alzheimer's Disease Center, Boston, MA; [7]Department of Neurology, Boston University School of Medicine, Boston, MA; [8]Brain Science Institute, Korea Institute of Science and Technology (KIST), Seoul, South Korea*

WP 543 **Analysis of Age- and Sex-Related Protein Stability Changes Brain Tissue Cell Lysates from a Mouse Model of Alzheimer's Disease**; Yun Tang[1]; Michael C. Fitzgerald[1]; *[1]Duke University, Durham, NC*

WP 544 **Development of a rapid LC-MS/MS method for determination of 13 organophosphorus pesticides and metabolites in human serum**; Maya Rae N Mugosa[1]; Tammy Jones-Lepp[1]; Erin N Toledano Strom[1]; Ruth Marfil-Vega[2]; Celica Cosmme[3]; Loren Gabriel Pasia[1]; Justin Miller[4]; Aaron Ritter[4]; Jefferson W Kinney[1]; Stephen Kurzyniec[2]; *[1]Pam Quirk Brain Health and Biomarker Laboratory ,Department of Brain Health, School of Integrated Health Sciences, University of Nevada Las Vegas, Las Vegas, Nevada; [2]Shimadzu Scientific Instruments, Columbia, MD; [3]University of Nevada Las Vegas, Kirk Kerkorian School of Medicine, Las Vegas, Nevada; [4]Cleveland Clinic Lou Ruvo Center for Brain Health, Las Vegas, Nevada*

WP 545 **Differential proteomics in enteroendocrine cells to investigate a brain axis model of Parkinson's disease**; Ying Yan[1]; Julia Balsamo[2]; Elizabeth N Bess[2]; Stephanie M Cologna[1]; *[1]University of Illinois Chicago, Chicago, IL; [2]University of California, Irvine, Irvine, CA*

WP 546 **Brain glycaproteomics and proteomics analyses reveal key glycated lysine residues of hallmark proteins pathologically associated with Alzheimer's disease**; Qin Fu[1]; Elizabeth T. Anderson[1]; Gary E. Gibson[2]; Sarah A. Flowers[3]; Sheng Zhang[1]; *[1]Proteomics and Metabolomics Facility, Cornell University, Ithaca, NY; [2]Weill Cornell Medicine, Burke Neurological Institute, White Plains, NY; [3]Department of Neuroscience, University of Virginia, Charlottesville, VA*

WP 547 **Characterizing Amyloidogenic Protein Oligomers by Native and Top-Down Mass Spectrometry**; Eileen Jacqueline Olivares[1]; Carter Lantz[2]; Rachel Loo[1]; Joseph A. Loo[1]; *[1]University of California, Los Angeles, Los Angeles, CA; [2]Texas A&M University, College Station, TX*

WP 548 **Mapping the human hippocampus using spatial tissue proteomics**; Johanna Tüshaus[1]; Lisa Abel[2]; Bernhard Kuster[1]; *[1]TU Munich, Freising, Germany; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

WP 549 **Molecular spatial distribution in transgenic rat model of Alzheimer's disease using MALDI MS imaging**; Tong Shen[1]; Pamela Lein[2]; Oliver Fiehn[1]; *[1]West Coast Metabolomics Center, University of California, Davis, Davis, CA; [2]Department of Molecular Biosciences, School of Veterinary Medicine, University of California, Davis, Davis, CA*

WP 550 **Risk assessment for dementia and Alzheimer's disease using plasma amyloid biomarker quantification by immunoprecipitation-mass spectrometry**; Jana Kindermans[1]; Germain Ulysse Busto[2, 3]; Christophe Hirtz[1]; Isabelle Carriere[2]; Karim Bennys[2, 3]; Laure-Anne Gutierrez[2]; Catherine Helmer[4]; Audrey Gabelle[2, 3]; Claudine Berr[2]; Sylvain Lehmann[1]; *[1]LBPC-PPC, Montpellier University, IRMB CHU Montpellier, INM INSERM, Montpellier, France; [2]INM, University of Montpellier, INSERM, Montpellier, France; [3]Memory Resource and Research Center, Department of Neurology, University of Montpellier Hospital, Montpellier, France; [4]University of Bordeaux, INSERM UMR U1219, Bordeaux Population Health (BPH) Research Centre, BORDEAUX, France*

WP 551 **Proteomic signatures of sex and social environment: a comparative analysis of the midbrain periaqueductal gray, hippocampus, and cortex**; Kristina Desch[1, 2]; Elena Kutsarova[1]; Petros Chalas[1]; Imke Wüllenweber[2]; Genesis Rosiles[1]; Vanessa Stempel[1]; Julian D. Langer[1, 2]; *[1]Max-Planck-Institute for Brain Research, Frankfurt am Main, Germany; [2]Max-Planck-Institute of Biophysics, Frankfurt am Main, Germany*

WP 552 **Profiling CDKL5-Dependent Phosphoproteome Landscape of Mouse Synaptosome and Hippocampus by DIA Mass Spectrometry**; Yi-Kai Liu[1]; Dayne Martinez[2]; Marco Hadisurya[1]; Zhaolan Zhou[2]; W. Andy Tao[1, 3, 4]; *[1]Department of Biochemistry, Purdue University, West Lafayette, IN; [2]Department of Genetics, University of Pennsylvania, Philadelphia, PA; [3]Department of Chemistry, Purdue University, West Lafayette, IN; [4]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN*

WP 553 **Applications of orthogonal label-free single-shot DIA platforms in understanding pathway heterogeneities in C9orf72 ALS using patient-derived astrocytes and microglia**; Mahmud Hossain[1]; Jaunetta Hill[1]; Steven Rodriguez[1]; Leonardo Rodrigues[1]; James Dodge[1]; Bailin Zhang[1]; Dhiman Ghosh[1]; *[1]Sanofi, Cambridge, MA*

WP 554 **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[1]; James Movius[1]; Aarun Hendrickson[1]; Asmit Kumar[2]; Ingrid Redford[1]; Jaden Le[1];

Jarrad Scarlett[1]; Kimberly Alonge[1]; Miklos Guttman[3]; [1]*University of Washington, Seattle, WA; [2]University of Washington, Seattle; [3]University of Washington, Seattle, WA*

WP 555 **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[1]; Avery M Runnebohm[1]; Whitney Smith-Kinnaman[1]; Emma H Doud[1]; Stephane Pelletier[1]; Amber L Mosley[1]; [1]*Indiana University School of Medicine, Indianapolis, IN*

WP 556 **An atlas of Histone H3.2 and H4 Proteoform of the Mouse Brain**; Meggie N. Young[1]; Bethany Taylor[2]; Tao Wang[3]; Laura Lavery[4]; Huda Zoghbi[2]; Nicolas L. Young[2]; [1]*Baylor College of Medicine, Houston, TX; [2]Baylor College of Medicine, Houston, Texas; [3]Fred Hutchinson Cancer Research Center, Seattle, WA; [4]Rice University, Houston, TX*

WP 557 **Quantitative proteomics of white matter brain tissue for the analysis of Alzheimer's disease**; Gennifer E Merrihew[1]; Aaron J. Maurais[1]; Jea Park[1]; Deanna Plubell[1]; Bo Wen[1]; William S Noble[1]; C Dirk Keene[2]; Thomas Montine[3]; Michael J. MacCoss[1]; [1]*University of Washington - Genome Sciences, Seattle, WA; [2]University of Washington - Laboratory Medicine and Pathology, Seattle, WA; [3]Stanford University - Pathology, Stanford, CA*

WP 558 **Sex-specific Differences in Distributions of Small Molecules in Brain Regions of Alzheimer's Disease Mouse Model using DESI-MSI**; BEHNAZ AKBARI[1]; Victoria L. Wendt[1]; Jitika Rajpoot[2]; Christina R. Ferreira[3]; Caitlin Randolph[2]; Connor H Beveridge[2]; Aditya Kangune[4]; Palak Manchanda[1]; Gaurav Chopra[2]; [1]*Purdue University, Department of Chemistry, West Lafayette, IN; [2]Purdue University Department of Chemistry, West Lafayette, IN; [3]Bindley Bioscience Center, Purdue University, West Lafayette, Indiana; [4]Purdue University, Department of Statistics, West Lafayette, IN*

WP 559 **Linking Soil Chemistry to Parkinson's Disease Pathogenesis: Novel Neurodegenerative Compounds from Streptomyces venezuelae**; Timothy J Bushman[1]; Osagie Emokpae[1]; Jennifer L Thies[1]; Lena Seyfarth[1]; Elizabeth Gokie[1]; Brandon J Kim[1]; Kim A Caldwell[1]; Lukasz Ciesla[1]; [1]*The University of Alabama, Tuscaloosa, AL*

WP 560 **Can Unique Biomarkers Be Identified for 'Exophers'? - An LCM-MS Study**; Megan Hong[1]; Rachel Loo[1]; Joseph Loo[1]; Gal Bitan[1]; Prashant Kaushal[1]; Mehdi Bouhaddou[1]; [1]*UCLA, Los Angeles, CA*

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WP 561 **Analysis of Posttranscriptional RNA Modifications with MetaMorpheus**; Isabella T Whitworth[1]; Nicholas E Bollis[1]; Mark Scalf[1]; Michael R Shortreed[1]; Lloyd M Smith[1]; [1]*University of Wisconsin-Madison, Madison, WI*

WP 562 **Developing LC-MS based Methods for Routine Quality Control Testing of Phosphoramidite Starting Materials for Oligonucleotide Therapeutics**; Rajeswari Lakshmanan[1]; Steve Rice[1]; Phil Olsen[1]; Dennis Rhodes[1]; Claus Rentel[1]; [1]*Ionis Pharmaceuticals, Inc., Carlsbad, CA*

WP 563 **Sequencing of Phosphorodiamidate Morpholino Oligomers by Hydrophilic Interaction Chromatography Coupled to Tandem Mass Spectrometry**; Mingming Wang[1]; Brian O'Day[1]; Brian Michaels[1]; Tao Wei[1]; Jurjus Jurayj[1]; Bao Zhong Cai[1]; [1]*Sarepta Therapeutics, Andover, MA*

WP 564 **Assessment of assay-related overdigestion in mRNA poly(A) analysis by LC-MS**; James Boslett[1]; Hannah Demirovic[2]; Janice Wei[1]; Miraslava Potapenko[1]; Oleg Jouravlev[1]; Fanyu Meng[1]; [1]*Pfizer, Pearl River, NY; [2]Stony Brook University, Stony Brook, NY*

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WP 566 **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[1]; Balasubrahmanyam Addepalli[2, 3]; Patrick A. Limbach[2]; [1]*University of Cincinnati, Cincinnati, OH; [2]University of Cincinnati, cincinnati, OH; [3]Waters Corporation, Milford, MA*

WP 567 **Nucleoside modification mapping by genome-independent universal mass exclusion list of unmodified oligonucleotides during LC-MS/MS**; Asif Rayhan[1]; Balasubrahmanyam Addepalli[2]; Patrick A. Limbach[2]; [1]*Universtiy of Cincinnati, Cincinnati, OH; [2]University of Cincinnati, cincinnati, OH*

WP 568 **The Addition of Transcriptomics to the Bead-enabled Accelerated Monophasic Multi-omics Method: A Step Toward Universal Sample Preparation**; Joshua D. Breidenbach[1, 2]; Emilio S. Rivera[1, 2]; Tara Harvey[1, 2]; Abigale S. Mikolitis[1, 2]; Chi-Yen Tseng[1, 2]; Claire K. Sanders[3]; Emilia A. Solomon[2]; Cheryl D. Gleasner[4]; Grace M. Thornhill[1, 2]; Kes A. Luchini[1, 2]; Brett R. Blackwell[1, 2]; Erick S. LeBrun[1, 2]; Phillip M. Mach[1, 2]; Jennifer F. Harris[5]; Jurgen G. Schmidt[1, 2]; Austin R. Anderson[1, 2]; Lauren K. Heine[1, 2]; Jessica A. Salguero[1, 2]; Salvator J. Palmisano[1, 2]; Francisca E. Rodriguez[1, 2]; Zachary J. Sasiene[1, 2]; Ethan M. McBride[1, 2]; Trevor G. Glaros[1, 2]; [1]*Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [2]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [3]Microbial and Biome Sciences Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [4]Genomics and Bioanalytics Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [5]Physical Chemistry and Applied Spectroscopy Group, Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM*

WP 569 **Development of a streamlined LC-HRMS/MS-based workflow for identification of mRNA sequence**; Camila A Ortega Ramirez[1]; Julio Hernandez Lopez[1]; Inna Koukhareva[1]; Khaled Yamout[1]; [1]*Trilink Biotechnologies, San Diego, CA*

WP 570 **Morpholino antisense oligonucleotides analyses using a compact matrix-assisted laser-desorption/ionization digital-ion-trap mass spectrometer (MALDI-DIT-MS)**; Yuko Fukuyama[1]; Sadanori Sekiya[1]; Shinichi Iwamoto[1]; Koichi Tanaka[1]; [1]*Shimadzu Corporation, Kyoto, Japan*

WP 571 **Investigating cyclic ion mobility as a means to boost coverage in the topdown sequencing of synthetic guide RNAs**; Catherine Tremblay[1]; Dale A Cooper-Shepherd[2]; Chris Knowles[3]; Michael Ruehl[4]; Christopher Gawlig[4]; James I. Langridge[5]; [1]*Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters Corporation, Newcastle, United Kingdom; [4]Biospring GmbH, Frankfurt am Main, Germany; [5]Waters Corporation, Wilmslow, United Kingdom*

WP 572 **SEC x IP Two-Dimensional LCMS for the Analysis of Non-Denatured and Denatured Cyclic-Peptide siRNAs in a Single Step**; Stilianos G. Roussis[1]; Kristine Nguyen[1]; Claus Rentel[1]; [1]*Ionis Pharmaceuticals, Inc., Carlsbad, CA*

WP 573 **Rapid Profiling of Impurities in Synthetic Oligonucleotides Using a Semi-Automated Data Analysis Workflow with ToF-MS**; Nick Pittman[1]; Ying Qing Yu[2]; Scott Berger[2]; Guillaume Bechade[2]; Kellen Delaney[2]; [1]*Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA*

WP 574 **Anion exchange chromatography fractionation of complex RNA mixtures for enhanced modification mapping via LC-MS/MS**; Cassandra Herbert[1]; Jennifer Kist[1]; Patrick A. Limbach[1]; [1]*University of Cincinnati, Cincinnati, OH*

WP 575 **Systematic Evaluation of Hydrophilic Interaction Liquid Chromatography Stationary Phases for Oligonucleotide Characterization by LC/MS**; Jordy J Hsiao[1]; Alex Apffel[1]; Lee Bertram[1]; Andrea Tripodi[2]; Andrew Coffey[2]; Ta-Chen Wei[3]; Connor Flannery[1]; [1]*Agilent Technologies, Santa Clara,* *CA; [2]Agilent Technologies Inc., Church Stretton, United Kingdom; [3]Agilent Technologies, Wilmington, DE*

WP 576 **Determination of Collision Cross-Sections of Nucleic Acids using an Orbitrap Mass Analyzer**; Jada N. Walker[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

WP 577 **A Quantitative Competitive Transcription and Adduct Bypass Assay of Transcriptional Inhibition and Mutagenesis by O2-Alkylthymidine Lesions**; Chen Wang[1]; Xiaomei He[1]; Yinan Wang[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

WP 578 **Global Analysis of Structured RNA-Protein Interactions using Stability-Based Mass Spectrometry Methods**; Morgan A. Bailey[1]; Justin G. Martyr[2]; Amanda E. Hargrove[1, 2]; Michael C. Fitzgerald[1, 2]; *[1]Department of Chemistry, Duke University, Durham, NC; [2]Department of Biochemistry, Duke University School of Medicine, Durham, NC*

WP 579 **Development of a SIM-based LCMS method for analysis of ribonucleoside mono-, di- and triphosphates and their mixtures**; Julio Hernandez Lopez[1]; Camila A Ortega[1]; Inna Koukhareva[1]; Khaled Yamout[1]; *[1]Trilink Biotechnologies, San Diego, CA*

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WP 581 **Rapid monitoring of the purification process of oligonucleotide impurities using a benchtop MALDI-TOF MS system**; Takashi Nishikaze[1]; Kosuke Uchiyama[1]; Risa Suzuki[2]; Junji Kawakami[3]; Takao Inoue[4]; Satoshi Obika[5]; Yoshihiro Hayakawa[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]SHIMADZU Corporation, Kawasaki, Japan; [3]Konan University, Kobe, Japan; [4]National Institute of Health Sciences, Kawasaki, Japan; [5]Osaka university, Osaka, Japan*

WP 582 **Identification and functional characterizations of DNA N2-alkylguanine-binding proteins**; Ting Zhao[1]; Xiaomei He[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

WP 583 **Quantitative Analysis of a GalNAc-siRNA Conjugate and Its Metabolites Using Two-Dimensional Liquid Chromatography Coupled with Tandem Mass Spectrometry**; Li Fang[1]; Peiyun An[1]; Jinlian Lu[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

WP 584 **Characterization of 3‘-poly(A)-tail length distribution in IVT-mRNA RNAse A/T1 double digestions using sliding windows deconvolution**; Alexander Boris Schwahn[1]; Ken Cook[2]; *[1]Thermo Fisher Scientific, Reinach, Switzerland; [2]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*

WP 585 **High-throughput LC/MS characterization of mRNA therapeutics using a fast DDA method on the Orbitrap Astral MS**; Tabiwang Arrey[1]; Angela Criscuolo[1]; Keeley Murphy[2]; Eugen Damoc[1]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Thermo Fisher Scientific, San Jose, CA*

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WP 589 **Targeted peptide quantification with small foot-print capillary LC-MS/MS**; Xiaoli Dong[1]; Matthew Morse[2]; Greg Ward[2]; Linfeng Wu[1]; Patrick Batoon[1]; *[1]Agilent, Santa Clara, CA; [2]Axcend, Provo, UT*

WP 590 **Quantitation of a glucagon-like peptide-1 (GLP-1) analog in rat plasma using an LC-MS/MS workflow**; Amy Knight[1]; Ebru Selen[1]; Rahul Baghla[1]; Eshani Galermo[1]; *[1]SCIEX, Redwood City, CA*

WP 591 **High-Throughput Characterization of Peptide Active Pharmaceutical Ingredient (API) Manufacturing Impurities by High-Resolution Ion Mobility Mass Spectrometry (HRIM-MS)**; Ashli R Simone[1]; Sumukh Ray[2]; Michelle English[1]; Greg Kilby[1]; *[1]MOBILion Systems, Chadds Ford, PA; [2]Bachem Americas, Inc., Vista, CA*

WP 592 **Quantitative Target Engagement for a KRAS G12C Inhibitor in FFPE Tumor Tissues using Immunoaffinity Capture 2D-LC-MRM**; Aiying Yu[1]; Jintang He[1]; Lingyao Meng[1]; Zhen Shi[1]; Emily Chan[1]; Thomas Hunsaker[1]; Jian Jiang[1]; Surinder Kaur[1]; Keyang Xu[1]; *[1]Genentech Inc, South San Francisco, CA*

WP 593 **Sensitive quantitation of glucagon-like peptide-1 (GLP-1) analog in rat plasma**; Tanya Gamble[1]; Ebru Selen[2]; Rahul Baghla[2]; Eshani Galermo[2]; *[1]SCIEX, Concord, ON; [2]SCIEX, Redwood City, CA*

WP 594 **Quantitative Analysis of Protein Expression and Oxidative Damage in E. coli Strains Lacking Key Antioxidant Enzymes**; Yanjia Zhang[1]; Sanjay Kumar Rohaun[2]; James Imlay[2]; Aaron Timperman[1]; *[1]University of Pennsylvania, Philadelphia, PA; [2]University of Illinois at Urbana-Champaign, Urbana, IL*

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WP 596 **Applying targeted mass spectrometry to pulsed SILAC for protein turnover and quantitative proteomics**; Brooke Brauer; *AstraZeneca, Waltham, MA*

WP 597 **Capillary blood devices comparison for small peptide detection (<2 kDa) by LC-HRMS in antidoping analysis**; Carlotta Stacchini[1]; Fabio Comunità[1]; Xavier De La Torre[1]; Daniel Jardines[1]; Francesco Botrè[1, 2]; *[1]Antidoping Laboratory FMSI, Rome, Italy; [2]University of Lausanne, Lausanne, Switzerland*

WP 598 **Systematic quantification of rare misreading events in the bacterial inner membrane**; Nicola S. Freyer[1]; Nilanjan Ghosh Dastidar[1]; Ingo Wohlgemuth[1]; Henning Urlaub[1, 2]; Marina V. Rodnina[1]; *[1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; [2]University Medical Center Göttingen, Göttingen, Germany*

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WP 600 **Thermo Instrument Application Programming Interface enables on-the-fly adjustment of FAIMS compensation voltages for large-scale internal standard triggered PRM**; Nathan T Wamsley[1]; Michael B Major[1]; Dennis Goldfarb[1]; *[1]Washington University in Saint Louis, St. Louis, MO*

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MacLean[2]; Jae Choi[3]; Bhavin Patel[3]; Ryan Bomgarden[3]; Eric Zaniewski[4]; Johannes Kreuzer[4]; Lecia V Sequist[4]; Wilhelm Haas[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of Washington - Genome Sciences, Seattle, WA; [3]Thermo Fisher Scientific, ROCKFORD, IL; [4]Massachusetts General Hospital (MGH), Charlestown, MA*

WP 602 **Targeted measurements enable robust quantitation of low-abundance proteins from single cells**; H. Lavender Lin[1]; Lilian R Heil[2]; Fernanda Salvato[2]; Philip M. Remes[2]; Cristina C. Jacob[2]; Amirmansoor Hakimi[2]; Tonya Pekar Hart[2]; Ryan T. Kelly[1]; *[1]Brigham Young University, Provo, UT; [2]ThermoFisher Scientific, San Jose, CA*

WP 603 **Interrogating the heart disease-relevant protein isoform landscape of smooth muscle cells using mass spectrometry**; Jennifer A Korchak[1]; Erin Jeffery[1]; Mayank Murali[1, 2]; Noah Perry[1]; Mete Civelek[1]; Gloria Sheynkman[1]; *[1]University of Virginia, Charlottesville, VA; [2]Broad Institute of MIT and Harvard, Cambridge, MA*

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WP 606 **Quantitative LC-MS/MS Analysis of Exogenously Administered Oxytocin in Pediatric Patients**; Jeff Jeppson[1]; Lee Winchester[1]; Anthony Podany[1]; Christopher Shaffer[1]; *[1]UNMC, Omaha, NE*

WP 607 **Mapping start codons of small open reading frames by N-terminomics approach**; Cuihong Wan; *Central China Normal University, Wuhan, China*

WP 608 **Inheritance in wet-dry cycling based Prebiotic Evolving Chemical Systems**; Kavita R Matange[1]; Vahab Rajaei[1]; Loren Dean Williams[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

WP 609 **Utilizing the power of the timsTOF Ultra for targeted PRM analysis**; Casey Powers[1]; Allis Chien[2]; Ryan Leib[2]; Fang Liu[2]; *[1]Stanford University, Stanford, CA; [2]Stanford University Mass Spectrometry, Stanford, California*

WP 610 **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[1]; Yunlong Zhao[1]; Yuan Mao[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Inc., Tarrytown, NY*

WP 611 **Charged-Surface Stationary Phase Improves Peptide Peak Shape in Low Ionic Strength Mobile Phases**; Benjamin Libert[1]; Barry Boyes[1]; Chuping Luo[1]; *[1]Advanced Materials Technology, Wilmington, DE*

WP 612 **Sub-Picogram Level Bio-Analytical Method for Quantification of Desmopressin in Human Plasma Using LCMS-8060NX**; Chaitanya Krishna Atmakuri[1]; Avinash B Gaikwad[1]; Yogesh G Arote[1]; *[1]ADC-Shimadzu Analytical India Pvt Ltd, NAVI MUMBAI, India*

WP 613 **Scout triggered MRM : a method to acquire large numbers of MRM without predefined retention time**; Holly Lee[1]; David Cox[1]; Yves Le Blanc[2]; *[1]SCIEX, Concord, ON; [2]SCIEX, Concord, On, ON*

WP 614 **Precise and accurate quantitation of critical host cell proteins (HCPs) using a targeted peptide mixture and LC-MS/MS analysis**; Noelia De Lama[1, 2]; Corentin Beaumal[1, 2]; Jae Choi[3]; Bhavin Patel[3]; Nikki Jarrett[3]; Kay Opperman[3]; Christine Carapito[1, 2]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, IPHC (UMR 7178), CNRS, Strasbourg, France; [2]Infrastructure Nationale de Protéomique ProFI – FR2048, Strasbourg, France; [3]Thermo Fisher Scientific, ROCKFORD, IL*

WP 615 **A Rapid Liquid Chromatography-Mass Spectrometry Quantitation of Somatostatin in Rat Plasma**; Yongjing He[1]; Zhenhua Jiang[1]; Lizhi Guo[1]; Nan Zhao[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

WP 616 **Comprehensive quantitation of the mitochondrial proteome with parallel reaction monitoring and real-time retention alignment**; Valerie N. Lynch[1]; Lilian R Heil[2]; Chris McGann[1]; Erik Bergstrom[1]; Philip M Remes[2]; Cristina C. Jacob[2]; Devin K Schweppe[1]; *[1]University of Washington - Genome Sciences, Seattle, WA; [2]ThermoFisher Scientific, San Jose, CA*

WP 617 **The power of the multi-attribute method in advancing novel modalities in process and product development**; Vamsikrishna Kandhi[1]; Keith Johnson[1]; *[1]Pfizer Inc., Andover, MA*

WP 618 **Optimizing DIA and PRM workflows for the Orbitrap Astral mass spectrometer**; Marcel Morgenstern[1, 2]; Benton J Anderson[1, 2]; Noah Michael Lancaster[1, 3]; Corinne Moss[1]; Margaret Lea Robinson[1]; Pavel Sinitcyn[4]; Joshua J Coon[1, 2, 3, 4]; *[1]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [2]National Center for Quantitative Biology of Complex Systems, Madison, WI; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [4]Morgridge Institute for Research, Madison, WI*

PROTEIN THERAPEUTICS: QUANTITATIVE ANALYSIS

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WP 619 **Double Immunocapture-LC/MS/MS Assay Method Development and Validation in Support of BI-X GLP Monkey Ocular Studies**; Bailuo Ren[1]; Yan Mao[1]; David Roos[1]; Kelly Coble[1]; *[1]Boehringer Ingelheim, Ridgefield, CT*

WP 620 **Nontraditional IC-LC/MS Method Development and Bioanalysis for On Demand Cytokines**; Emily Werth[1]; Elsy Philip[1]; Tammy Bigwarfe[1]; Kelly Coble[1]; *[1]Boehringer Ingelheim, Ridgefield, CT*

WP 621 **A Spectra library assisted workflow for host cell protein detection and quantitation in recombinant peptide drug products by CapLC-HRMS/MS**; Cung N Thawng[1]; Cynthia Sommers[1]; Eric Pang[2]; David A Keire[1]; Hongbin Zhu[3]; *[1]U.S. FDA, St Louis, MO; [2]U.S. Food and Drug Administration, Silver Spring, MD; [3]U.S. FDA, Saint Louis, MO*

WP 622 **An Approach for Multi Attribute Monitoring of Bi-Specific Antibodies Employing Capillary Electrophoresis and Intact Mass Spectrometry**; Nancy Fernandes; *Lonza, Portsmouth, NH*

WP 623 **Implementing Microflow LC-MS/MS for Quantification of Antibody-drug Conjugates and Biotherapeutic Proteins During Early Drug Discovery and Development**; Joshua B Powers[1]; Moo-jin Suh[1]; *[1]AstraZeneca, Gaithersburg, MD*

WP 624 **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[1]; Mojibola Fowowe[1]; Vishal Sandilya[1]; Botheina Ghandour[2]; Firas Kobeissy[2, 3]; Nadine Darwiche[2]; Yehia Mechref[1]; *[1]Chemistry and Biochemistry Department, Texas Tech University, Lubbock, TX; [2]Department of Biochemistry and Molecular Genetics, American University of Beirut, Beirut, Lebanon; [3]Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Morehouse School of Medicine, Atlanta, GA*

WP 625 **Antibody guanidination: an alternative antibody internal standard approach to antibody quantification in canine plasma using IA LC-MS/MS**; Drupadkumar Acharya[1]; Henry Li[1]; Wei Tong[1]; Laura Letendre[1]; *[1]Boehringer Ingelheim Animal Health USA Inc., North Brunswick, NJ*

WP 626 **Develop and Validate a Universal LC-MS/MS Assay to Quantify Succinylated Gelatin in Human Plasma to Support BE Studies**; Yuhuan Ji[1]; Changgang Li[1]; Changjian Zhao[1]; Min Meng[1]; Laixin Wang[1]; *[1]Resolian China, Chongqing, China*

WP 627 **Multi-Omics Investigation of Biotherapeutic Expressing CHO Cell Lines In Fed Batch Bioreactors**; Charles Eldrid[1]; Ellie Hawke[1]; Lee A Gethings[2]; John Raven[3]; Richard Lock[2]; Joanna Watson[1]; Alan Dickson[1]; James I. Langridge[2]; Leon Pybus[3]; Andrew Pitt[1]; Perdita Barran[1]; *[1]University of Manchester, Manchester, United Kingdom; [2]Waters*

Corporation, Wilmslow, United Kingdom; [3]FUJIFILM Diosynth Biotechnologies UK, Billingham, United Kingdom

WP 628 **Coupling Enrichment and Depletion Methods with FAIMS-MS for Enhanced Host Cell Protein Identification in Biotherapeutic Development**; Christopher Sauer[1]; Abby J. Chiang[2]; Elsa Gorre[1]; Andrew D Mahan[1]; Hirsh Nanda[1]; *[1]Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania; [2]Protein Metrics, LLC, Cupertino, CA*

WP 629 **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[1]; Anisha Rai[1]; Shuyu Hou[1]; Tian-Sheng Lu[1]; *[1]Medpace, Cincinnati, OH*

WP 630 **Automated 96-well desalting and collision induced unfolding analysis of biotherapeutics**; Michael R Armbruster[1]; Amanda Cicali[1]; Tyler Somerville[1]; Nicole A Rivera-Fuentes[1]; Youngseo Na[2]; Alyssa Erlenbeck[1]; Anna Schwendeman[3]; Brandon T Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, Michigan; [2]Department of Medicinal Chemistry, University of Michigan, Ann Arbor, MI; [3]Department of Pharmaceutical Sciences, University of Michigan, Ann Arbor, MI*

WP 631 **Development of a novel middle-up HILIC-MS method for intra-domain free thiol localization and quantitation in therapeutic monoclonal antibodies**; Xin Wang[1]; Xiaoxiao Huang[1]; Shunhai Wang[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Inc., Tarrytown, NY*

WP 632 **Intact Mass Analysis for the Quantitation of Free Subunits Observed in Antibody-based Proteins**; Kyoung-Soo Choi[1]; Pooja Madhav Raju[1]; Helen Zou[1]; John Patrick[1]; Steven Pomerantz[1]; Tun Liu[1]; Richard Huang[1]; *[1]Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania*

WP 633 **A Single, Integrated Software Platform for LC/MS-based Multi-Attribute Method (MAM) Approaches, with Automated Review**; Aude Tartiere[1]; Can Cui[2]; Catherine Evans[3]; Stephen Kok[1]; Yaarub Musa[3]; Arnd Brandenburg[3]; *[1]Genedata Inc, San Francisco, CA; [2]Genedata Inc., Lexington, Massachusetts; [3]Genedata AG, Basel, Switzerland*

WP 634 **Regulated Bioanalysis for Large Peptide/Small Protein Quantitation in Matrix by LC–MS: Can We Detect Intact or Digested Peptide?**; Moucun Yuan[1]; Kumar Shah[1]; Gang Xu[1]; Gus Hui[1]; M. Shane Woolf[1]; William R. Mylott Jr. [1]; *[1]PPD, part of Thermo Fisher Scientific, Richmond, VA*

WP 635 **Identification and Quantitation of Heterodimers in Co-Formulated Monoclonal Antibody Cocktails: From Sample Treatment Strategies to Native SEC-MS Analysis**; Wenjing Peng[1]; Yuetian Yan[1]; Victoria C. Cotham[1]; Shunhai Wang[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Inc., Tarrytown, NY*

WP 636 **Development of an LC-MS/MS Assay for Quantitative Analysis of the Biotherapeutic Protein that Overcomes the ADA Impact in Human Serum**; Gang Xu[1]; Joe Palandra[2]; Kumar Shah[1]; Moucun Yuan[1]; Gus Hui[1]; William R. Mylott Jr. [1]; M. Shane Woolf[1]; Mike Baratta[2]; *[1]PPD, part of Thermo Fisher Scientific, Richmond, VA; [2]Takeda Development Corporation, Americas, Cambridge, MA*

WP 637 **Localization of PTMs on Multi Specific antibody through Middle down analysis by Microfluidic Chip-Based Integrated icIEF-UV/MS technology**; Kristen Nields[1]; Hirsh Nanda[2]; Scott Mack[3]; Zoe Zhang[4]; Mariam S ElNaggar[3]; Megan E. Sharma[2]; Riley Schaeffer[2]; Robert Hepler[2]; *[1]Janssen Biopharmaceticals, Springhouse, PA; [2]Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania; [3]SCIEX, Fremont, CA; [4]SCIEX, Redwood City, CA*

WP 638 **De Novo Sequencing and Assembly of Multiclonal Nanobodies**; Qingyang Xiao[1]; Sujun Li[1]; Haixu Tang[1]; *[1]Indiana University, Bloomington, IN*

WP 639 **Exploiting Isotope Resolution of Intact Protein Mass Spectra with Gábor Transform for Improved Multi-Protein Deconvolution and Accurate, Automated Antibody Quantitation**; Kayd L. Meldrum[1]; Andrew K. Swansiger[1]; Meghan Daniels[1]; Crystal Kirmiz Cody[2]; David L. Wong[2]; Mike Knierman[2]; Xi Qiu[2]; John Sausen[2]; Anthony D. Maus[3]; Paula M. Ladwig[3]; Maria A. V. Willrich[3]; James S. Prell[1, 4]; *[1]University of Oregon, Eugene, OR; [2]Agilent Technologies, Santa Clara, CA; [3]Mayo Clinic, Rochester, MN; [4]Materials Science Institute, University of Oregon, Eugene, OR*

WP 640 **Nano LC/MS based quantitative assessment of the processing of a novel conditionally active bispecific T-cell engager in monkey plasma**; Yipei Zhang[1]; Mark G. Qian[1]; Linlin Dong[1]; *[1]Takeda Development Corporation, Americas, Cambridge, MA*

WP 641 **Interlaboratory study for characterizing NISTmAb by microfluidic chip-based integrated imaged capillary isoelectric focusing (icIEF)-UV/MS**; Mariam S ElNaggar[1]; Kristen Nields[2]; Kristine F Parson[3]; Anita P Liu[4]; Xiaoping Z He[5]; Tony Cozzolino[6]; James Ingersoll[7]; Steven Chow[1]; Rita Nichiporuk[1]; Jose-Luis Gallegos-Perez[6]; Zhenjiu Liu[5]; Zac VanAernum[4]; Margo Wilson[3]; Riley Schaeffer[2]; Seung-Yong Jung[1]; Jackie Le[1]; Rashmi Madda[7]; Megan E. Sharma[2]; Daniel Zorzon[7]; Fred Mannarino[7]; Sisi Huang[5]; Michael Merriman[7]; Alexander Petrov[1]; Scott Mack[1]; Daniel French[7]; John Orlet[8]; Jingwen Ding[1]; Alcenir Soares[7]; Chelsea Leonce[2]; Jennifer Chui[1]; Matthew Heindel[7]; Tom Lerch[8]; Haichuan Liu[7]; Thomas Powers[9]; Wei Chen[1]; Lien Kwan[7]; Vincent Vang[1]; Johan Hermansson[7]; Melissa Anderson[8]; Tristan Williams[7]; *[1]SCIEX, Fremont, CA; [2]Janssen Research and Development, Spring House, PA; [3]FUJIFILM Diosynth Biotechnologies USA, Inc, Morrisville, NC; [4]Merck, Kenilworth, NJ; [5]Pfizer, Chesterfield, MO; [6]Sciex, Framingham, MA; [7]SCIEX, Redwood City, CA; [8]Pfizer Inc., Chesterfield, MO; [9]Pfizer Inc, Chesterfield, MO*

WP 642 **Quanifying epitope-specific affinities of naturally acquired antibodies to a malaria protein using native mass spectrometry**; Daniel Ferrer Vinals[1]; Duong T. Bui[2]; Mohammad R. Hoque[1]; Eliana Arango[3]; Amanda Maestre[3]; Lara K. Mahal[2]; Stephanie K. Yanow[1]; John S. Klassen[2]; *[1]School of Public Health, University of Alberta, Edmonton, AB; [2]Department of Chemistry, University of Alberta, Edmonton, AB; [3]Grupo Salud y Comunidad, Facultad de Medicina, Universidad de Antioquia, Medellin, Colombia*

WP 643 **New tools for biologics analyses and QC: the Shredder and S-Trap Turbo MAM**; Stefan Loroch[1, 2]; Sandra Wilson[1]; Alexandre Zougman[3]; John P Wilson[1]; *[1]Protifi, LLC, Fairport, NY; [2]Ruhr-University Bochum, Bochum, Germany; [3]University of Leeds, Leeds, United Kingdom*

PROTEINS: GENERAL AND MEMBRANE
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WP 644 **Mass Spectrometric Identification of Invasion Receptors on Red Blood Cell Precursors for the Malaria Parasite Plasmodium vivax**; Jessica S Molina[1]; Daniel Roeth[1]; Manuel Alfonso Patarroyo[2]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA; [2]Fundación Instituto de Inmunología de Colombia, Bogotá, Colombia*

WP 645 **Enhanced Signal Processing Methods for Membrane Protein Collision Induced Unfolding Analysis**; Iliana Levesque[1]; Kristine F. Parson[2]; Sarah M. Fantin[3]; Aniruddha Panda[4]; Kallol Gupta[4]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, Michigan; [2]FUJIFILM Diosynth Biotechnologies USA, Inc, Morrisville, North Carolina; [3]Hanover College, Hanover, Indianna; [4]Yale University, West Haven, CT*

WP 646 **Development of Mass Spectrometry Grade Membrane Protein Standard**; Alyson Jesionowski[1]; Leigh Foster[1]; Aaron McBride[1]; Joanna Geddes[1]; Kay Opperman[1]; Barbara Kaboord[1]; Bhavin Patel[1]; Weijing Liu[2]; Yuqi Shi[2]; Rosa Viner[2]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, San Jose, CA*

WP 647 **Studies of Aquaporin-0 Lipid Binding in the Bovine Lens via Native Mass Spectrometry**; Carla V.T. O'Neale[1]; Sophie R. Harvey[2]; Vicki H. Wysocki[2]; Kevin L. Schey[1]; *[1]Vanderbilt University, Nashville, TN; [2]The Ohio State University, Columbus, OH*

WP 648 **Analysis of Membrane Proteins under Native and Denaturing Conditions Using Capillary Electrophoresis Coupled to High-Resolution Mass Spectrometry**; Noah Gould[1]; Yunfan Gao[1]; Michal Gregus[1]; Kendall R Johnson[1]; Anne-Lise Marie[1]; Alexander R. Ivanov[1]; *[1]Northeastern University, Boston, MA*

WP 649 **A comparison of sample preparation, data acquisition and data processing workflows for untargeted bottom-up plasma proteomics**; Carina Lima[1]; Leanne Ohlund[1]; Kevin Ly[2]; Maxim Isabelle[2]; Victoria Miller[2]; Hugo Gagnon[2]; Lekha Sleno[1]; *[1]UQAM, Montreal, QC; [2]Allumiqs, Sherbrooke, QC*

WP 650 **Unbiased characterization of GPCRs spatiotemporal activities revealed novel receptor trafficking and signaling signatures**; Qiongyu Li[1]; Benjamin Polacco[1]; Martin Gordon[1]; Trupti Patil[1]; Aaron Marley[1]; Prachi Khare[1]; Jiewei Xu[1]; Xiaofang Zhong[1]; Emily Blythe[1]; Aliza Ehrlich[1]; Kirsten Obernier[1]; Nevan Krogan[1]; Mark Von Zastrow[1]; Ruth Huttenhain[1, 2]; *[1]University of California, San Francisco, San Francisco, CA; [2]Stanford University, Palo Alto, CA*

WP 651 **Characterization of Insect Sperm Nuclear Basic Proteins by Liquid Chromatography – Tandem Mass Spectrometry**; Melissa R Leyden[1]; Donald F. Hunt[1]; Jeffrey Shabanowitz[1]; *[1]University of Virginia, Charlottesville, VA*

WP 652 **Unveiling the SEA Domain Self-Cleavage of GPR110 and its Impact on GAIN Domain Autoproteolysis: Insights from Quantitative Mass Spectrometry**; Bill Huang[1]; Hee-Yong Kim[1]; *[1]NIAAA/NIH, Rockville, MD*

WP 653 **A lipid vesicle ion mobility-mass spectrometry platform uncovers how membrane protein-lipid organization at the synaptic membrane drives ultrafast neurotransmitter release**; Aniruddha Panda[1]; Iliana Levesque[2]; Anna L. Duncan[3]; Jean N.D. Goder[1]; Frederic Pincet[4]; Brandon T Ruotolo[5]; Kallol Gupta[1]; *[1]Department of Cell Biology, Yale University, West Haven, CT; [2]Department of Chemistry, University of Michigan, Ann Arbor, MI; [3]Department of Chemistry, Aarhus University, Aarhus, Denmark; [4]Laboratoire de Physique de l'Ecole Normale Supérieure, ENS, CNRS, Université PSL, Sorbonne Université, Université Paris-Cité, Paris, France; [5]Department of Chemistry, University of Michigan, Ann Arbor, Michigan*

WP 654 **Analysis of Whole Cell Yeast Lysates by Charge Detection Mass Spectrometry**; Nick Rommel[1]; Adam Anthony[1]; David Clemmer[1]; *[1]Indiana University, Bloomington, IN*

WP 655 **Characterizing Ligand Binding to the AmtB/GlnK Complex using Direct Mass Technology**; Jared Hampton[1]; Robert L. Schrader[1]; Robert Rider[1]; Smriti Kumar[1]; Carter Lantz[1]; David H Russell[1]; *[1]Texas A&M University, College Station, TX*

WP 656 **A high-throughput proteome-wide platform for capturing membrane proteins in their native environment for structural and functional studies**; Caroline Brown[1]; Snehasish Ghosh[1]; Yansheng Liu[2]; Moitrayee Bhattacharyya[2]; Kallol Gupta[1]; *[1]Yale School of Medicine, Department of Cell Biology, New Haven, CT; [2]Yale School of Medicine, Department of Pharmacology, New Haven, CT*

WP 657 **Whole proteome analysis of endothelial cells in response to catecholamine stimulation using an untargeted approach**; Arnar Ingi Vilhjalmsson[1]; Óttar Rolfsson[1]; *[1]University of Iceland, Reykjavik, Iceland*

WP 658 **nanoCSC reveals novel insight into the surfaceome of primary human cardiomyocytes in heart failure**; Roneldine Mesidor[1]; Melinda Wojtkiewicz[1]; Michelle Waknitz[1]; Rebekah L Gundry[1]; *[1]University of Nebraska Medical Center, Omaha, NE*

WP 659 **HiBiT Protein Tagging System for Quantitative Study of Protein Dynamics at Endogenous Levels**; Virginia Kincaid[1]; Christopher Eggers[1]; Mike Rosenblatt[1]; Brock Binkowski[1]; Marjeta Urh[1]; *[1]Promega Corporation, Madison, WI*

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WP 660 **Enrichment of Methylated Peptides Using Strong Cation Exchange with an Optimized Salt Gradient**; Amanda Ziegler[1]; Jessica M Conforti[1]; Hadden K Swanzy[1]; Charli S Worth[1]; Joseph H Taube[1]; Elyssia S Gallagher[1]; *[1]Baylor University, Waco, TX*

WP 661 **PTMeXchange species specific PTM builds: Meta-analysis of datasets and dissemination of high-quality PTM data for community use**; Kerry A Ramsbottom[1]; Ellen Boswell[1]; Oscar M Camacho[1]; Shireen Al-Momani[1]; Ananth Prakash[2]; Yasset P Riverol[2]; Zhi Sun[3]; Deepti J Kundu[2]; Emily Bowler-Barnett[2]; Maria Martin[2]; Jun Fan[2]; Eric W Deutsch[3]; Juan Antonio Vizcaíno[2]; Andrew R. Jones[1]; *[1]University of Liverpool, Liverpool, United Kingdom; [2]European Bioinformatics Institute, Cambridge, United Kingdom; [3]Institute for Systems Biology, Seattle, Washington*

WP 662 **Deciphering the Notch signalling pathway using magnetic beads coupled with delta ligands and quantitative phosphoproteomics**; Michael Saynisch[1, 2]; Levent Marcel Oelmez[1, 2]; Marcus Krüger[1, 2]; Luisa Schmidt[1, 2]; Jan-Wilm Lackmann[1, 2]; Stefan Müller[1, 2]; *[1]University of Cologne, Cologne, Germany; [2]CECAD (Cluster of Excellence in Cellular Stress Responses in Aging-Associated Diseases), Cologne, Germany*

WP 663 **Assessment of aging profile of archaeological animal bone collagen in terms of glutamine deamidation using mass spectrometry**; Takashi Nakazawa[1]; Masaru Miyagi[2]; Kazuki Kawahara[3]; Seiji Kadowaki[4]; Yoshihiro Nishiaki[5]; *[1]Nara Women's University, Nara, Japan; [2]Case Western Reserve University, Cleveland, Ohio; [3]Osaka Univeristy, Suita, Japan; [4]Nagoya University, Nagoya, Japan; [5]The University of Tokyo, Bunkyo-ku, Japan*

WP 664 **Ethanol-induced post-translational acetylation alters hepatic metabolism in mice**; Mirjavid Aghayev[1]; Sergeui Ilchenko[1]; Victor Lufi[1]; Jack Mathis[1]; Megan McMullen[2]; Hannah Marchuk[3]; Tsung-Heng Tsai[4]; Guofang Zhang[3]; Laura Nagy[2]; Takhar Kasumov[1]; *[1]Northeast Ohio Medical University, Rootstown, OH; [2]Cleveland Clinic, Cleveland, OH; [3]Duke University, Durham, NC; [4]Kent State University, Kent, OH, 44240*

WP 665 **Automated and Robust Identification of Scrambled Disulfide Bonds in Biotherapeutics**; Stephen Kok[1]; Aude Tartiere[1]; Can Cui[2]; Catherine Evans[3]; Yaarub Musa[3]; Arnd Brandenburg[3]; *[1]Genedata Inc, San Francisco, CA; [2]Genedata Inc., Boston, MA; [3]Genedata AG, Basel, Switzerland*

WP 666 **Mapping functions of diphthamide biosynthetic enzymes using multiple proteomic approaches**; Lauren Mazurkiewicz[1]; Amy Weeks[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 667 **HinT erases AMPylation and GMPylation from proteins revealed by mass spectrometric analysis**; Yanping Qiu[1]; Heenam Park[1]; Chieh-Hsiang Tan[1]; Baiyi Quan[1]; Paul W. Sternberg[1]; Tsui-Fen Chou[1]; *[1]Caltech, Pasadena, CA*

WP 668 **Definitive Identification of Sulfation in an Antibody SEFL1 Motif by High Resolution Mass Spectrometry with Site Identification by EThcD MS/MS**; John H. Robinson[1]; Shuai Wu[1]; Iain D.G. Campuzano[1]; *[1]Amgen Inc., Thousand Oaks, CA*

WP 669 **Formation of Cys-TMT from Interaction of iodoTMT0 with Cysteine Residues Alkylated by N-Ethylmaleimide (NEM)**; Jian Cai[1]; Ming Song[2, 3]; Ming Li[1]; Michael Merchant[1]; Frederick Benz[4]; Craig McClain[2, 3, 4, 5, 6]; Jon Klein[1, 5]; *[1]1. Division of Nephrology and Hypertension, Department of Medicine, University of Louisville School of Medicine, Louisville, Kentucky; [2]2. Division of Gastroenterology, Hepatology and Nutrition, Department of Medicine, University of Louisville School of Medicine, LOUISVILLE, Kentucky; [3]3. Hepatobiology and Toxicology Center, University of Louisville, LOUISVILLE, Kentucky; [4]4. Department of Pharmacology and Toxicology, University of Louisville School of Medicine, Louisville, Kentucky; [5]5. Robley Rex Veterans Affairs*

Medical Center, Louisville, Kentucky; [6]6. Alcohol Research Center, University of Louisville, Louisville, Kentucky

WP 670 **An Integrated Multi-PTM Workflow for Simultaneous Analysis of Phosphorylation, Glycosylation, Acetylation and Ubiquitination**; Yuanwei Xu[1]; T. Mamie Lih[2]; Lijun Chen[2]; Hui Zhang[2, 3]; *[1]Johns Hopkins University, Baltimore; [2]Johns Hopkins University School of Medicine, Baltimore city, MD; [3]Johns Hopkins University, Baltimore, MD*

WP 671 **Mapping Post-Translational Modifications of the oncoprotein MEK1 by Tandem Top-down Proteomics**; Raveena Gupta[1]; Jared O Kafader[1]; Bryon S Drown[1]; Paul J Hergenrother[2]; Craig M Horbinski[3]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]University of Illinois Urbana-Champaign, Champaign, IL; [3]Northwestern University, Feinberg School of Medicine, Chicago, IL*

WP 672 **Untargeted phosphoproteomics reveals unique biomarkers of colorectal cancer**; Ashima Mehta[1]; Adam D. Richardson[1]; Ethan Stancliffe[1]; Monil Gandhi[1]; Gary J. Patti[1, 2]; *[1]Panome Bio, Saint Louis, MO; [2]Washington University in Saint Louis, St. Louis, MO*

WP 673 **Mass Spectrometry Analysis of Intact Glycopeptides from Formalin-Fixed Paraffin-Embedded Prostate Tissue Samples**; Abel Bermudez[1]; Fernando Garcia-Marques[2]; Hongjuan Zhao[1]; Dalin Zhang[2]; James D. Brooks[2]; Sharon J Pitteri[2]; *[1]Stanford University, Palo Alto, CA; [2]Stanford University, Stanford, CA*

WP 674 **Protein search engine using databases annotated with proteoforms from UniprotKB**; Titus H Jung[1]; Casimir Bamberger[2]; Salvador Martinez De Bartolome[3]; Robin Park[4]; John R. Yates III[2]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Scripps Research, La Jolla, CA; [3]Yatiri Biosciences, San Diego, CA; [4]Bruker Daltonics GmbH & Co. KG, Billerica, MA*

WP 675 **Quantitative analysis of non-histone lysine methylation sites and lysine demethylases in breast cancer cell lines**; Christine A Berryhill[1]; Emma H Doud[1]; Amber L Mosley[1]; Evan M Cornett[1]; *[1]Indiana University School of Medicine, Indianapolis, IN*

WP 676 **Structural basis for polyglutamate chain initiation and elongation by TTLL family enzymes**; Kishore K Mahalingan[1]; Keith Keenan[1]; Madeleine Strickland[2]; Yan Li[3]; Yanjie Liu[4]; Haydn L Ball[5]; Martin E. Tanner[4]; Nico Tjandra[2]; Antonina Roll-Mecak[1, 2]; *[1]Cell Biology and Biophysics Unit, Porter Neuroscience Research Center, National Institute of Neurological Disorders and Stroke,, Bethesda, MD; [2]Biochemistry & Biophysics Center, National Heart, Lung and Blood Institute, Bethesda, MD; [3]Proteomics Core Facility, NINDS, Bethesda, MD; [4]Department of Chemistry, University of British Columbia, Vancouver, British Columbia; [5]University of Texas Southwestern Medical Center, Protein Chemistry Technology Center, Dallas, TX*

WP 677 **Phosphoproteomics profiling reveals the kinome regulated signaling pathways in human dendritic cells treated with immunomodulators under IFN-g triggered inflammatory stress**; Cristina C Clement[1]; Rajesh K Soni[2]; Laura Santambrogio[1]; *[1]Weill Cornell Medicine, New York, NY; [2]Proteomics and Macromolecular Crystallography Shared Resource, Herbert Irving Comprehensive Cancer Center, Columbia University Irving Medical Center, New York, NY*

WP 678 **Application of sub-unit intact mass to screen antibody chemical liabilities in early-stage discovery**; Xiaohua Liu[1]; Sagar Kathuria[1]; Nancy Yongjia Gong[1, 2]; Zachary Beamer[3]; *[1]Sanofi, Cambridge, MA; [2]Rutgers University, New Brunswick, NJ; [3]Sanofi, Framingham, MA*

WP 679 **Optimization and Characterization of Disulfide Linkages in the Complex Cysteine Engineered Stapled scFV for Bispecific Antibodies**; Abby J. Chiang[1]; Elsa Gorre[2]; Alexander N. Barnakov[2]; Christopher Sauer[2]; Reiko Kiyonami[3]; Min Du[3]; Andrew Mahan[2]; Hirsh Nanda[2]; *[1]Protein Metrics, LLC, Cupertino, CA; [2]JOHNSON AND JOHNSON, Spring House, PA; [3]Thermo Fisher Scientific, Lexington, MA*

PROTEOMICS: INTACT PROTEINS AND TOP DOWN ANALYSIS I

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WP 680 **Stem cell differentiation analysis by top-down proteomics using capillary zone electrophoresis-ion mobility spectrometry-mass spectrometry**; Jorge A. Colon-Rosado[1]; Zhaoran Zhang[1]; Yuan Wang[1]; Liangliang Sun[1]; *[1]Michigan State University, East Lansing, MI*

WP 681 **Residue-specific backbone cleavage of intact proteins directed by photoactive alpha radicals**; Lin He[1]; Ryan R. Julian[1]; *[1]University of California, Riverside, Riverside, CA*

WP 682 **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[1]; Katharina E. Meijboom[2]; Robert H Brown Jr. [2]; Jeffrey N. Agar[1]; *[1]Barnett Institute of Chemical and Biological Analysis, Dept. of Chemistry and Chemical Biology, Northeastern University, Boston, MA; [2]Department of Neurology, University of Massachusetts Medical School, Worcester, Massachusetts*

WP 683 **Leveraging gas-phase fractionation and ion-ion reactions for the spatial analysis of the intact human proteome up to 70 kDa**; Jake T Kline[1]; Jingjing Huang[2]; Christopher Mullen[3]; Joseph B Greer[4]; David Bergen[3]; Michael W Belford[3]; Cornelia L Boeser[3]; Vlad Zabrouskov[3]; Kenneth R Durbin[4]; Graeme C McAlister[3]; Rafael D Melani[3]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific – 355 River Oaks Pkwy, San Jose, California; [4]Proteinaceous, Inc., Evanston, IL*

WP 684 **Improved Top-down Sequencing of Protein Ions via Mobility Enhanced Pseudo-MS3Collisional Activation**; Katherine A Graham[1]; Nicholas B. Borotto[1]; *[1]University of Nevada Reno, Reno, NV*

WP 685 **Unified LC-DAD-MS method for accurate and reproducible analysis of miscellaneous intact protein samples in a core facility setting**; Serge Chesnov[1]; Ralph Schlapbach[1]; Paolo Nanni[1]; *[1]Functional Genomics Center Zurich – ETH Zurich/University of Zurich, Zurich, Switzerland*

WP 686 **Application of 210Po charge reduction to facilitate the characterization of intact proteins by 193 nm ultraviolet photodissociation**; Sean D Dunham[1]; Jennifer Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

WP 687 **Sequence Analysis of Proteins enhanced by TIMS-Enabled Next-Generation MALDI Top-Down Sequencing using a Dedicated Software Workflow**; Arndt Asperger[1]; Mariangela Kosmopoulou[2]; Dodge Baluya[3]; Detlev Suckau[1]; *[1]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [2]Fasmatech Science and Technology, Athens, Greece; [3]Bruker Scientific LLC, San Jose, CA*

WP 688 **An Expanded RAS Proteoform Landscape Provided by Top-Down Analysis of Malignant Cell Lines**; Grace M. Scheidemantle[1]; Robert A. D'Ippolito[1]; Kanika Sharma[1]; Nicole Fer[1]; Brian Smith[1]; Mackenzie Meyer[1]; Scott Eury[1]; Abigail Neish[1]; Katie Powell[1]; Vanessa Wall[1]; William Burgan[1]; Dominic Esposito[1]; Anna E. Maciag[1]; Frank McCormick[1, 2]; Dwight V. Nissley[1]; Caroline DeHart[1]; *[1]Frederick National Laboratory for Cancer Research, Frederick, MD; [2]Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA*

WP 689 **Fast Top-Down Analysis via Orbitrap and Astral Analyzers**; Hamish Stewart[1]; Tabiwang Arrey[1]; Eugen Damoc[1]; Max Hoek[1]; Christian Hock[1]; *[1]Thermo Fisher Scientific, Bremen, Germany*

WP 690 **Capillary Electrophoresis-Mass Spectrometry with Cationic Polymer Coating for Reproducible Measurement of Proteoforms**; Guangyao Gao[1]; Qianjie Wang[1]; Liangliang Sun[1]; *[1]Michigan State University Department of Chemistry, East Lansing, MI*

WP 691 **Mapping Top-Down Mass Spectrometry Data onto Three-Dimensional Protein Structures for Elucidation of Structural Proteoform Insights**; Jessie A. Bolger[1]; Kenneth R. Durbin[1]; Matthew T. Robey[1]; Ryan T. Fellers[1, 2]; *[1]Proteinaceous, Evanston, IL; [2]Northwestern University, Evanston, IL*

WP 692 **The Development of Optimized Cyclic Ion Mobility-Mass Spectrometry Methods for Native Top-Down Proteomics**; Ryan K Schroeder[1]; Devin Makey[1]; Carolina Rojas Ramírez[2]; Brandon T Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, Michigan; [2]Department of Pathology, University of Michigan, Ann Arbor, Michigan 48109, United States, Ann Arbor, Michigan*

WP 693 **In-Depth Characterization of Protein Kinase Complexes by Top-Down Mass Spectrometry**; Hsin-Ju Chan[1]; Boris Krichel[2]; Emily A. Reasoner[1]; Man-Di Wang[1]; Ying Ge[1, 2, 3]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Cell and Regenerative Biology, Madison, WI; [3]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*

WP 694 **Multidimensional Sample Pre-Fractionation Workflow for Deep Middle-Down Proteomics**; Ayako Takemori[1]; Philipp T. Kaulich[2]; Andreas Tholey[2]; Nobuaki Takemori[1]; *[1]Ehime University, Toon, Japan; [2]Christian-Albrechts-Universität zu Kiel, Kiel, Germany*

WP 695 **FLASHViewer: a web application with a configurable layout for top-down mass spectrometry data visualization**; Jihyung Kim[1, 2]; Andrew Almaguer[3]; Kyowon Jeong[1, 2]; Jaekwan Kim[4]; Axel Walter[1, 2]; Wonhyeuk Jeong[5]; Oliver Kohlbacher[1, 2, 6]; *[1]University of Tübingen, Tübingen, Germany; [2]Institute for Bioinformatics and Medical Informatics, University of Tubingen, Tubingen, Germany; [3]jambit GmbH, Stuttgart, Germany; [4]Omics Research Center, Sejong, South Korea; [5]Yale School of Medicine, New Haven, CT; [6]Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany*

WP 696 **FLASHIda:FAIMS - Intelligent Data Acquisition for FAIMS enabled Top-Down Proteomics**; Tom D. Müller[1, 2]; Kyowon Jeong[1, 2]; Philipp T. Kaulich[3]; Andreas Tholey[3]; Oliver Kohlbacher[1, 2, 4]; *[1]Applied Bioinformatics, Department for Computer Science, University of Tübingen, Tübingen, Germany; [2]Institute for Bioinformatics and Medical Informatics, University of Tübingen, Tübingen, Germany; [3]Systematic Proteome Research & Bioanalytics, Institute for Experimental Medicine, Christian-Albrechts-Universität zu Kiel, Kiel, Germany; [4]Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany*

WP 697 **Top-Down Protein Sequencing of Simple Protein Mixtures combining Liquid Chromatography and Cyclic Ion Mobility TOF Mass Spectrometry**; Marie LEY[1]; Victor COCHARD[1]; Véronique LEGROS[1]; Jean-Michel CAMADRO[1]; Guillaume CHEVREUX[1]; *[1]ProteoSeine CNRS, Institut Jacques Monod, Université Paris Cité, Paris, France*

WP 698 **Probing Non-Covalent Interactions Between Proteins and Small Molecules with Photoactivated Radical Dissociation**; Evan E Hubbard[1]; Ryan R. Julian[1]; *[1]University of California, Riverside, Riverside, CA*

WP 699 **Improved top-down analysis of antibody subunits using the Omnitrap-Orbitrap-Booster platform**; Camille Garcia[1, 2, 3]; Konstantin O. Nagornov[4]; Athanasios Smyrnakis[5]; Anton N. Kozhinov[4]; Dimitris Papanastasiou[5]; Yury O. Tsybin[4, 6]; Julia Chamot-Rooke[1]; *[1]Institut Pasteur, Paris, France; [2]Université Paris Cité, Paris, France; [3]CNRS UAR2024, Paris, France; [4]Spectroswiss, Lausanne, Switzerland; [5]Fasmatech, Athens, Greece; [6]Spectrotech, Lyon, France*

WP 700 **Native Mass Spectrometry and Top-Down MS of Acyl-Lysine Modified Protein Complexes**; Yi Qiao[1]; Boyu Zhao[1]; Rachel Loo[2]; Joseph A. Loo[1]; *[1]University of California, Los Angeles, Los Angeles, CA; [2]University of California Los Angeles, Los Angeles, CA*

WP 701 **Top-down proteomics analysis of pg-level cell lysate using spray-capillary CE-FAIMS-MS**; Samin Anjum[1]; Zhitao Zhao[2]; Kellye A Cupp-Sutton[1]; Si Wu[1]; *[1]The University of Alabama, Tuscaloosa, AL; [2]University of Oklahoma, Norman, OK*

WP 702 **Revealing Cerezyme Glycoforms by Native Capillary Zone Electrophoresis Mass Spectrometry (nCZE-MS)**; Danye Qiu[1]; Hucong Jiang[1]; Tongdan Wang[1]; Jincui Huang[1]; *[1]WuXi Biologics, Shanghai, China*

WP 703 **Advanced Top-Down Data Analysis with MetaMorpheus**; Nicholas Bollis[1]; Katherine B Henke[2]; Michael R Shortreed[3]; Lloyd M Smith[3]; *[1]University of Wisconsin Madison, Madison, WI; [2]Yale School of Medicine, New Haven, CT; [3]University of Wisconsin-Madison, Madison, WI*

WP 704 **Enhancing Top-Down Mass Spectrometry Intact Protein Characterization through Aggregation of Multimodal Fragmentation Data**; Ken Durbin[1]; Matthew T. Robey[2]; Ryan T. Fellers[2]; Joseph B. Greer[2]; Bryan P. Early[2]; Daisha Utley[2]; *[1]Proteinaceous, Evanston, IL; [2]Proteinaceous, Inc., Evanston, IL*

WP 705 **Top-down Proteomics to Monitor Post-translational Protein Arginylation in Cell Systems**; Zongtao Lin[1]; Richard M Searfoss[1]; Xingyu Liu[1]; Axe Xie[1]; Emily Zahn[1]; Joanna M Gongora[1]; Rashmi Karki[1]; Bibhuti Bhusana Palai[1]; Daniel Ramirez[1]; Benjamin Garcia[1]; *[1]Washington University in St. Louis, St. Louis, MO*

WP 706 **Combining Top-Down and Bottom-Up Mass Spectrometry Paves the Way for High Throughput Polyclonal Antibody Sequencing**; Lei Xin[1]; Baozhen Shan[1]; Chao Peng[2]; Jun Ma[2]; Shuyang Zhang[1]; Zihao Wang[1]; Wenting Li[1]; *[1]Bioinformatics Solutions Inc., Waterloo, ON; [2]BaizhenBio Inc., Wuhan, China*

WP 707 **Capillary Zone Electrophoresis-Mass Spectrometry Reveals Histone Modification Patterns Change in Isogenic SW480 and SW620 Cell Lines**; Fei Fang[1]; Brian D Fries[2]; Amanda Hummons[2]; Liangliang Sun[1]; *[1]Department of Chemistry, Michigan State University, East Lansing, MI; [2]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH*

WP 708 **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[1]; Somak Ray[1]; Jeffrey N. Agar[1]; *[1]Northeastern University, Boston, MA*

WP 709 **Benchmarking A Visual Acuity Ion Classifier for MS/MS Deconvolution and Identification of Native Membrane Proteins In Vitro**; Adrian L Guthals[1]; Wonhyeuk Jung[2]; Aniruddha Panda[2]; Blake Hakkila[1]; Stephanie Sturgeon[1]; Timothy Djang[3]; Alex Gavrilenko[4]; Jhenya Gavrilenko[4]; Panos Iatrou[4]; Stelios Gkegkas[4]; Derrill Sturgeon[4]; Rachel Franklin[1]; Yury V. Vasilev[1]; Diana Oppenheimer[1]; Joseph Meeuswen[1]; Joseph Beckman[5]; Kallol Gupta[2]; *[1]Agilent Technologies, Corvallis, Oregon; [2]Yale School of Medicine, New Haven, CT; [3]Agilent Technologies, Santa Clara, CA; [4]Devicepros, Boston, USA, MA; [5]Oregon State University, Corvallis*

WP 710 **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[1]; Ruben Szabo[2]; Kenneth R. Durbin[3]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]University of Debrecen, Debrecen, Hungary; [3]Proteinaceous, Inc., Evanston, IL*

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WP 711 **Variance from sequential multi-‘omic extractions impact biological interpretation of viral disease model**; Molly Soper-Hopper[1]; Colt Capan[1]; Hyoungjoo Lee[1]; Ryan D Sheldon[1]; *[1]Van Andel Institute, Grand Rapids, MI*

WP 712 **Complementary ion quantification enables accurate multiplexing on the Orbitrap Astral**; Alex Johnson[1]; Martin Zeller[2]; Hamish Stewart[2]; Graeme McAlister[3]; Martin Wühr[1]; *[1]Princeton University, Princeton, NJ; [2]Thermo Fisher Scientific, Bremen, Germany; [3]ThermoFisher Scientific, San Jose, CA*

WP 713 **ProteomeIit 1.0: User-friendly and comprehensive software package for MS-based proteomics data analysis**; Ana Rita Colaço[1]; David Oliver Schlessinger[1]; Michael Wierer[1]; *[1]Proteomics Research Infrastructure, Novo*

Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark

WP 714 **Nascent proteomics reveals divergent contributions of 40 translation initiation factors to shaping the proteome**; Toman Bortecen[1, 2]; Robert Kalis[3]; Johannes Zuber[3]; Jeroen Krijgsveld[1, 4]; *[1]German Cancer Research Center (DKFZ), Heidelberg, Germany; [2]Heidelberg University, Heidelberg, Germany; [3]Institute of Molecular Pathology (IMP), Vienna, Austria; [4]Heidelberg University, Medical Faculty, Heidelberg, Germany*

WP 715 **Melanoma cells develop vemurafenib resistance through epitranscriptomic regulation**; Shiyuan Guo[1]; Tianyu F. Qi[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

WP 716 **Understanding early proteomic response of Saccharomyces cerevisiae to different oxidants using label-free comparative proteomics analysis**; Debasish Ghosh[1]; Khadiza Zaman[2]; Laszlo Prokai[2]; Vladimir Shulaev[1]; *[1]UNIVERSITY OF NORTH TEXAS, Denton, TX; [2]University of North Texas Health Science Center, Department of Pharmacology and Neuroscience,, Fort Worth, Texas*

WP 717 **A Proteome-wide Comparison of TMT-based and DIA-based Datasets Using the Orbitrap Astral Mass Spectrometer**; Yuchen He[1]; Joao A. Paulo[1]; Steven P. Gygi[1]; *[1]Harvard Medical School, Boston, MA*

WP 718 **Species-deconvolved proteomics enables accurate identification and quantification of cancer and stromal proteins in patient-derived xenografts**; Shuo Qian[1]; Han Liu[2]; Shichen Shen[2]; Jun Qu[1, 2]; *[1]Roswell Park Comprehensive Cancer Center, Buffalo, NY; [2]SUNY at Buffalo, Buffalo, NY*

WP 719 **A multi-year longitudinal harmonization of quality controls in mass spectrometry proteomics core facilities**; Cristina Chiva[1, 2]; Roger Olivella[1, 2]; An Staes[3, 4, 5]; Teresa Mendes Maia[3, 4, 5]; Francis Impens[3, 4, 5]; Simon Devos[3, 4, 5]; Christian Panse[6, 7]; Karel Stejskal[8, 9, 10]; Karl Mechtler[8, 9, 10]; Thibaut Douché[11]; Mariette Matondo[11]; Bérangère Lombard[12]; Damarys Loew[12]; Mandy Rettel[13]; Dominic Helm[13, 14]; Andrea Schuhmann[15]; Anna Shevchenko[15]; Paolo Nanni[6]; Eduard Sabidó[1, 2]; *[1]Centre de Regulació Genòmica, Barcelona Institute of Science and Technology (BIST), Barcelona, Spain; [2]Univeristat Pompeu Fabra, Barcelona, Spain; [3]VIB Proteomics Core, Ghent, Belgium; [4]VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; [5]Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; [6]Functional Genomics Center Zurich ETHZ/UZH, Zürich, Switzerland; [7]Swiss Institute of Bioinformatics (SIB), Lausanne, Switzerland; [8]Research Institute of Molecular Pathology (IMP), Vienna Biocenter (VBC), Vienna, Austria; [9]IMBA Institute of Molecular Biotechnology of the Austrian Academy of Sciences, Vienna Biocenter (VBC), Vienna, Austria; [10]Gregor Mendel Institute (GMI), Austrian Academy of Sciences, Vienna BioCenter 7 (VBC, Vienna, Austria; [11]. Institut Pasteur, Université Paris Cité, Proteomics Platform, Mass Spectrometry for Biology Unit, Paris, France; [12]Institut Curie, PSL Research University, Centre de Recherche, CurieCoreTech Mass Spectrometry Proteomics, Paris, France; [13]Proteomics Core Facility, European Molecular Biology Laboratory, Heidelberg, Germany; [14]Proteomics Core Facility, German Cancer Research Center (DKFZ), Heidelberg, Germany; [15]Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany*

WP 720 **Comparing gas phase enabled spectral library generation and library free DIA based phosphoproteomics**; Dongmei Zhang[1]; Ling Li[1]; Belinda Willard[1]; *[1]Cleveland Clinic, Cleveland, OH*

WP 721 **Low-input Proteomic Analysis Unveils Critical Pathways Underlying the Role of IL-4 and/or IL-13 on Human Mast Cells**; Bo Yang[1]; Kai-Ting Shade[1]; Preeti Bais[1]; Alexandra Hicks[1]; Hendrik Wesseling[1]; Bailin Zhang[1]; *[1]Sanofi, Cambridge, MA*

WP 722 **Dynamic TRPV2 ion channel proximity proteomics links calcium flux to cellular adhesion factors NCAM and L1CAM in neurite outgrowth**; Robyn J. Eisert[1]; Pamela Gallo[2]; Elaine Mihelca[2]; Gary A. Bradshaw[1]; Marian Kalocsay[3]; Vera Moiseenkova-Bell[2]; *[1]Harvard Medical School, Boston, MA; [2]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; [3]MD Anderson Cancer Center, Houston, Texas*

WP 723 **Profiling of Aging-induced Proteome Alternation in Calbindin- and Calretinin-positive Neurons in Mouse Hippocampus with a micoPOTS Platform**; Yen-Chen Liao[1]; Jeong Han Lee[2]; Sarah M Williams[1]; Lisa M Bramer[3]; Ljiljana Paša-Tolić[1]; Ying Zhu[1]; Ebenezer N. Yamoah[2]; *[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; [2]Department of Physiology and Cell Biology, School of Medicine, University of Nevada, Reno, NV; [3]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA*

WP 724 **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[1]; Shichen Shen[2]; Shihan Huo[2]; Min Ma[1]; Sailee Rasam[2]; Jun Qu[1, 2]; *[1]Roswell Park Comprehensive Cancer Center, Buffalo, NY; [2]SUNY at Buffalo, Buffalo, NY*

WP 725 **Deciphering Molecular mechanisms: Neuropeptide Signaling Pathways Explored Through Proteomic Analysis in Rat brain tissue**; Meera Asokan[1]; Abby Askins[2]; Luis Natividad[2]; *[1]University of Texas Austin, Austin, TX; [2]University of Texas at Austin, Austin, Texas*

WP 726 **Proximity labeling together with LC-MS/MS for interrogating the proximity proteome of METTL1**; Zhongwen Cao[1]; Xingyuan Chen[1]; Quanqing Zhang[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

WP 727 **Label-Free Quantitation with High Accuracy and Precision on a Single-Cell Scale with Orbitrap Astral Mass Spectrometer: An Inter-laboratory Study**; Anna Pashkova[1]; Jenny Ho[2]; Tabiwang N. Arrey[1]; Florian Marty[3]; Eugen Damoc[1]; Min Huang[4]; Sonja Radau[5]; Shio Watanabe[6]; Pedro Navarro[7]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [3]Thermo Fisher Scientific, Reinach, Switzerland; [4]Thermo Fisher Scientific, Shanghai, China; [5]Thermo Fisher Scientific, Dreieich, Germany; [6]Thermo Fisher Scientific, Yokohama, Japan; [7]Thermo Fisher Scientific, Bremen, Germany*

WP 728 **Harmonization of sample preparation and acquistion methods enables world-wide method transfer of proteomics workflows**; Jan Muntel[1]; Sandra Schär[2]; Luca Raess[2]; Christopher Below[2]; Roland Bruderer[2]; Jakob Vowinckel[2]; Nigel Beaton[1]; *[1]Biognosys Inc, Newton, MA; [2]Biognosys AG, Schlieren, Switzerland*

WP 729 **Deciphering the Proteomic Molecular Signatures of Traumatic Brain Injury in Serum and CSF by LC-MS/MS**; Vishal Sandilya[1]; Mojgan Atashi[1]; Thu Nguyen[1]; Joy O Solomon[1]; Md Mostofa Al Amin Bhuiyan[1]; Cristian D Gutierrez-Reyes[1]; Waziha Tasnim Purba[1]; Mojibola Fowowe[1]; Judith Ijeoma Nwaiwu[1]; Firas Kobeissy[2]; Stefania Mondello[3]; Ava M Puccio[4]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas; [2]Morehouse School of Medicine, Atlanta, Georgia; [3]University of Messina, Messina, Italy; [4]University of Pittsburgh, Pittsburgh, PA*

WP 730 **Use targeted proteomics analysis of key pathways to optimize cell culture media and feeds for Chinese Hamster Ovary cells**; Km Shams Ud Doha[1]; Martin Ciganda[1]; Chengjian Tu[1]; Didar Asik[1]; Jaime S Goldfuss[1]; Scott Jacobia[1]; Andy M Campbell[1]; *[1]Thermo Fisher Scientific, Grand Island, NY*

WP 731 **Double Immunoprecipitation (dIP) Trapping and Proteomics Mass Spectrometry to Discover Substrates of HDAC1 Involved in Sickle Cell Anemia**; Eric T.J Davis[1];

Urvashi Thongam[2]; Jennell White[2]; Mary K H Pflum[2]; [1]*Wayne State University, Detroit, MI;* [2]*Wayne State University, Detroit , MI*

WP 732 **A semi-automated SP3 sample preparation method for high throughput screening of in vivo BioID labeling on an Orbitrap Astral**; Greg Waitt[1]; Jaebin Kim[2]; Lucio Schiapparelli[2]; Scott Soderling[2]; Erik Soderblom[1, 2]; [1]*Proteomics and Metabolomics Core Facility, Duke University School of Medicine, Durham, NC;* [2]*Department of Cell Biology, Duke University School of Medicine, Durham, NC*

WP 733 **Evaluation of different lysine specific peptidases for MS-based proteomics**; Tanveer Singh Batth[1]; Cristina Hernandez Rollan[1]; Morten Nørholm[2]; Jesper Velgaard Olsen[1]; [1]*Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark;* [2]*NNF Center for Biosustainability, Denmark Technical University, Lyngby, Denmark*

WP 734 **Evaluation and optimization of FAIMS-based gas phase fractionation for increased DIA spectral library coverage on an Orbitrap Astral**; Tricia Ho[1]; Erik Soderblom[1]; [1]*Proteomics and Metabolomics Core Facility, Duke University School of Medicine, Durham, NC*

WP 735 **Expanding TMTpro reagents to 32-plex for high-throughput quantitative proteomics on Orbitrap platforms**; Dustin Frost[1]; Joao A. Paulo[2]; Steven P. Gygi[2]; Karsten Kuhn[3]; Ian Pike[3]; Ryan Bomgarden[1]; [1]*Thermo Fisher Scientific, Rockford, Illinois;* [2]*Harvard Medical School, Boston, MA;* [3]*Proteome Sciences, London, United Kingdom*

WP 736 **Toward Global Estimation of Endoplasmic Reticulum Import Efficiency via Sec61 Blockade and Proximity Labeling Mass Spectrometry**; Ziqi Lyu[1]; Joseph C. Genereux[1]; [1]*University of California, Riverside, Riverside, CA*

WP 737 **Protein identification and quantitation using scanning data-independent acquisition (DIA)**; Wen Jin[1]; Leroi DeSouza[1]; Alina Dindyal-Popescu[1]; Doug Simmons[1]; [1]*SCIEX, Concord, ON*

WP 738 **Exploring Drought Tolerance: Comparative Proteomics of Different Brassica rapa Plant Genotypes Using LFQ**; Brandon Anselmo Saiz[1]; Benjamin Conrad Romanjenko[1]; Carmela Rosaria Guadagno[1]; Brent E. Ewers[1]; Franco Basile[1]; [1]*University of Wyoming, Laramie, WY*

WP 739 **Applications and characterization of a new deuterium-enhanced TMTpro 32-plex reagent set for sample multiplexing**; Nathan Zuniga[1]; Dustin Frost[2]; Karsten Kuhn[3]; Ryan Bomgarden[2]; Ian Pike[3]; Steven P. Gygi[1]; Joao A. Paulo[1]; [1]*Harvard Medical School, Boston, MA;* [2]*Thermo Fisher Scientific, Bannockburn, IL;* [3]*Proteome Sciences, London, United Kingdom*

WP 740 **An in-depth investigation into plasma proteomic studies using DIA mass spectrometry and affinity-based platforms**; Aron Phong[1]; Balazs Szoke[1]; Benoit Lehallier[1]; Scott Lohr[1]; Sara Ahadi[1]; [1]*Alkahest Inc., San Carlos, CA*

WP 741 **Exploring whether Retrotranslocation During ER-Associated Protein Degradation is Affected by Proteasome Inhibition**; Qiqi Lin[1]; Ziqi Lyu[1]; Jasmine Castellanos[1]; Joseph Genereux[1]; [1]*University of California, Riverside, Riverside, CA*

WP 742 **Quantitative proteomic analysis of the protein levels involved in the maturation of the mammalian oocytes**; Piotr Suder[1]; Paulina Kret[1]; Wieslawa Mlodawska[2]; Igor Kotsan[1]; Anna Bodzon-Kulakowska[1]; [1]*AGH University of Krakow, Krakow, Poland;* [2]*University of Agriculture, Cracow, Poland*

WP 743 **Label-free quantitative proteomic analysis of spinal cord after morphine treatment**; Przemyslaw Mielczarek[1, 2]; Anna Bodzon-Kulakowska[3]; Jolanta H. Kotlinska[4]; Jerzy Silberring[3]; [1]*AGH University, Krakow, Poland;* [2]*Polish Academy of Sciences, Krakow, Poland;* [3]*AGH Univeristy of Krakow, Krakow, Poland;* [4]*Medical University of Lublin, Lublin, Poland*

WP 744 **Comparative proteome quantification reveals novellongevity regulators in IIS pathway ofC. elegans**; LANG DING; *Baylor College of Medicine, Houston, TX*

WP 745 **Protein Mistargeting Triggers a Cytosolic Quality Control Mechanism that Sorts Proteins Based on Thermodynamic Stability**; Jasmine Castellanos[1]; Joseph Genereux[2]; Khanh Nguyen[1]; [1]*University of California, Riverside, Riverside, CA;* [2]*University of California Riverside, Riverside, CA*

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WP 746 **Investigating Proteomic Changes Induced by Young Plasma Transfusion in the Recovery of Traumatic Brain Injury in Mice**; Wen-Chen Chen[1]; Wei-Che Chang[1]; Hsiao-Wei Chen[1]; Guo-Jen Huang[1]; Yi-Ting Chen[1]; [1]*Chang Gung Memorial University, Tao-yuan City, Taiwan*

WP 747 **Deep Lung Proteome Analysis of Bronchopulmonary Dysplasia Using TIMS TOF Ultra and 480 Exploris**; Daniela M Schlatzer[1]; Mark R Chance[1]; Anantha Krishnan Harijith[1, 2]; Filipa Blasco Tavares Pereira Lopes[1]; Tara Sudhadevi[1]; Matthew Willetts[3]; Diego Assis[3]; [1]*Case Western Reserve University, Cleveland, OH;* [2]*University Hospitals, Cleveland, OH;* [3]*Bruker Daltonics, Billerica, MA*

WP 748 **Proteomic Stability in Archival Formalin-Fixed and Paraffin-Embedded (FFPE) Tissue Sections Stored on Glass Slides by Mass Spectrometry**; Anqi Tu[1]; Beom-Jun Kim[1]; Nicolas Giraldo[1]; Chris Richardson[1]; David Chain[1]; Steve Sweet[1]; Yeoun Jin Kim[1]; Andrew Chambers[1]; [1]*AstraZeneca, Gaithersburg, MD*

WP 749 **iCAB: an insitu cell-type specific proteome analysis method using antibody-mediated biotinylation**; Taekyung Ryu[1]; Seok-Young Kim[1]; Thujitha Thuraisamy[1]; Jisu Shin[1]; Yura Jang[1]; Tae-In Kam[1, 2]; Chan-Hyun Na[1]; [1]*Johns Hopkins University School of Medicine, Baltimore, MD;* [2]*Korea Advanced Institute of Science and Technology, Daejeon, South Korea*

WP 750 **Pushing the limits of deep proteome analysis in muscle tissue**; Bingnan Zhao[1]; Noah M Lancaster[1, 2]; Katherine A Overmyer[1, 3, 4]; Perla Geara[5]; Jeffrey F. Dilworth[5]; Joshua J Coon[1, 2, 3, 4]; [1]*Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI;* [2]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [3]*Morgridge Institute for Research, Madison, WI;* [4]*National Center for Quantitative Biology of Complex Systems, Madison, WI;* [5]*Department of Cell and Regenerative Biology, Madison, WI*

WP 751 **Molecular Profiling of KCNT1 Mouse Model with ASO Treatment**; Fangxu Sun[1]; Fergal Casey[1]; Sijia Wu[1]; Yuqing Liu[1]; Thomas Carlile[1]; Paymaan Jafar-nejad[2]; Jing Wu[3]; Imran Quraishi[3]; Maysam Pedram[3]; Leonard K. Kaczmarek[3]; Viet Nguyen[1]; [1]*Biogen, Cambridge, MA;* [2]*Ionis Pharmaceuticals, Inc., Carlsbad, CA;* [3]*Yale University, New Haven, CT*

WP 752 **Laser Ablation Sampling for Formalin Fixed Paraffin Embedded Mouse Lung Tissue Proteomics**; Blessing Chisom Egbejiogu[1]; Come J. Thieulent[1]; Mariano Carossino[1]; Kermit K. Murray[1]; [1]*Louisiana State University, Baton Rouge, LA*

WP 753 **Profiling Protein-Protein Interactions in the Human Brain by Refined Co-Fractionation Mass Spectrometry**; Dong-Geun Lee[1]; Him Shrestha[1]; Junmin Peng[1]; [1]*St.Jude Children's Research Hospital, Memphis, TN*

WP 754 **Proteome changes during skin wound healing in healthy humans of different ages**; Alexey Lyashkov[1]; Ceereena Ubaida-Mohien[1]; Linda Zukley[1]; Shepherd H. Schurman[1]; Mary Kaileh[1]; Arsun Bektas[1]; Yevgeniya Lukyanenko[1]; Ruin Moaddel[1]; Julián Candia[1]; Chee Chia[1]; [1]*NIA/NIH, Baltimore, MD*

WP 755 **Aging Signatures Analyzing Human Lung Tissues Across the Lifespan by Data-Independent Acquisition: from Infancy to the Elderly**; Jacob Rose[1]; Joanna Bons[1]; Delphine Beaulieu[2]; Mark Watson[1]; John Sembrat[2]; Oliver Eickelberg[2]; Melanie Koenigshoff[2]; Birgit Schilling[1]; [1]*Buck*

Institute for Research on Aging, Novato, CA; [2]Center for Lung Aging and Regeneration, Division of Pulmonary Allergy Critical Care and Sleep Medicine, University of Pittsburgh, Pittsburgh, PA

WP 756 **Rapid tissue proteome profiling with trapped ion mobility mass spectrometry**; Felix Rudolf Schneidmadel[1]; Denys Oliinyk[1]; Andreas Will[1]; Phillip Köcher[1]; Florian Meier-Rosar[1]; *[1]Uniklinikum Jena, Functional Proteomics, Friedrich-Schiller-Univeristät, Jena, Germany*

WP 757 **Azo-Enabled Extracellular Matrix Proteomics for High-throughput Quantitative Analysis of Lung Tissue**; Anna G Towler[1]; Yanlong Zhu[2]; Timothy Aballo[3]; Kevin Buck[4]; Elizabeth Bayne[4]; Vanessa Morales-Tirado[5]; Yupeng (David) He[6]; Yu Tian[5]; Ying Ge[3, 4]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; [3]Department of Cell and Regenerative Biology, Madison, WI; [4]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [5]AbbVie Inc., Worcester, MA; [6]AbbVie Inc., North Chicago, IL*

WP 758 **Automated high-throughput proteomic analysis of stored blood cells from a large cohort of non-domestic felids**; Kevin L Schauer[1]; Kevin Yang[1]; Amirmansoor Hakimi[1]; Eugen Damoc[2]; Lily AB Parkinson[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Brookfield Zoo, Chicago Zoological Society, Brookfield, IL*

WP 759 **In situ, cell-type-specific proteome analysis using antibody-mediated biotinylation in mouse midbrains with Parkinson's disease**; Taekyung Ryu[1]; Seok-Young Kim[1]; Jae-Jin Song[1]; Tae-In Kam[1, 2]; Chan-Hyun Na[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD; [2]Korea Advanced Institute of Science and Technology, Daejeon, South Korea*

WP 760 **Characterizing Rat Placental/Amniotic Fluid Proteome: Toward Discovery of Placental Opioid Enhancing Factor (POEF) by Gel Electrophoresis and Bottom-up Proteomics**; Troy D Wood[1]; Brynn Nelson[1]; Alexandra Izydorczak[1]; Howell Phillips[1]; Jean DiPirro[2]; Mark Kristal[1]; Alexis Thompson[1]; *[1]University at Buffalo, Buffalo, NY; [2]Buffalo State University, Buffalo, NY*

WP 761 **Investigating ischemia and reperfusion-induced organ damage in severe cardiac arrest: A Comprehensive proteomics perspective**; Ju Yeon Lee[1, 2]; Muhammad Shoaib[3]; Jin-Woong Choi[4]; Jong Hwan Shin[4]; Rishabh C Choudhary[5]; Kei Hayashida[5]; Seunguk J Baek[6]; Santiago Miyara[5]; Jaewoo Choi[7]; Lance B Becker[3, 5, 8]; Junhwan Kim[3, 5, 8]; *[1]Korea Basic Science Institute, Cheongju, South Korea; [2]University of Science and Technology, Daejeon, South Korea; [3]Donald and Barbara Zucker School of Medicine, Hempstead, New York; [4]Korea Basic Science Institute, Cheongju, South Korea; [5]Feinstein Institute for Medical Research, Manhasset, New York; [6]Johns Hopkins University, Baltimore, MD; [7]Oregon State University, Corvallis, Oregon; [8]North Shore University Hospital, Manhasset, New York*

WP 762 **dia-PASEF proteomic analysis of HNSCC tumor and stroma enriched sections from FFPE samples prepared with laser capture microdissection**; Matthew Willetts[1]; Aswini Panigrahi[2]; Diego Assis[1]; Radoslav Goldman[2]; Allison Hunt[3]; Thomas P Conrads[3]; *[1]Bruker Scientific, LLC, Billerica, MA; [2]Georgetown University, Washington Dc, DC; [3]Women's Health Integrated Research Center, Annandale, VA*

WP 763 **A Deep Proteome and Protein Complex Analysis of Human Kidney Aging and Diseases**; Thao Nguyen[1]; Niclas Olsson[1]; Leanne J.G. Chan[1]; Wenzhou Li[1]; Phil Seitzer[1]; Aleksandr Gaun[1]; Edward L. Huttlin[1, 2]; Daigoro Hirohama[3]; Katalin Susztak[3]; Fiona McAllister[1]; *[1]Calico Life Sciences, South San Francisco, CA; [2]Department of Cell Biology, Harvard Medical School, Boston, MA; [3]Renal, Electrolyte, and Hypertension Division, Department of Medicine, University of Pennsylvania Perelman School of Medicine, Philadelphia, PA*

WP 764 **Unlocking the proteomic potential of FFPE tissues with BeatBox and iST: A xylene-free, high-throughput workflow for in-depth proteome analysis**; Brianne Nunez[1]; Katharina Limm[2]; Silvia Wuertenberger[2]; Katrin Hartinger[2]; Jonathan R Krieger[3]; Nils A. Kulak[2]; *[1]PreOmics, Billerica, MA; [2]PreOmics, Planegg/Martinsried, Germany; [3]Bruker Canada Ltd, Milton, ON*

WP 765 **High-throughput, streamlined processing workflow of formalin-fixed paraffin-embedded (FFPE) tissue yielding up to 10,000 proteins per sample**; Moe Haines[1]; John Thorup[1]; Simone Gohsman[1]; Lilian Heil[2]; Lia Abarzua[3]; Sameer Vasantgadkar[3]; Chelsea Newton[4]; Dan Rohrer[4]; Galen Hostetter[4]; D. R. Mani[1]; Michael A. Gillette[1]; Steven A. Carr[1]; Shankha Satpathy[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Covaris, LLC, Woburn, MA; [4]Van Andel Research Institute, Grand Rapids, MI*

WP 766 **Location! Location! Location! Deep topographic proteomics from tissue culture to a human brain tumor**; Simon Davis[1]; Yixin Shi[2]; Olaf Ansorge[2]; Philip Charles[2]; Stephen Taylor[2]; Roman Fischer[2]; *[1]University of Oxford, Oxford, United Kingdom; [2]University of Oxford, UK, Oxford, United Kingdom*

WP 767 **A Protocol Fast-Tracking Sample Preparation for Proteomics of Formalin Fixed Paraffin Embedded Tumor Tissues**; Lancia N.F. Darville-Bowleg[1]; John H. Lockhart[1]; Sudhir Putty Reddy[1]; Bin Fang[1]; Victoria Izumi[1]; Theresa A. Boyle[1]; Eric B. Haura[1]; Elsa R. Flores[1]; John M. Koomen[1]; *[1]Moffitt Cancer Center, Tampa, FL*

WP 768 **Comprehensive Analysis of FFPE Sections through Mass Spectrometry-Based Proteomics in a Fully Automated Workflow**; Paola Pisano[1]; Jonathan Samuel Achter[2]; Emma Maria Åhrman[1]; Katarzyna Izabela Wozniak[1]; Michele Puglia[1]; Irina Pozdnyakova[1]; Cristina Gil Gonzalez[1]; Alicia Lundby[2]; Michael Wierer[1]; *[1]Proteomics Research Infrastructure, Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark; [2]Department of Biomedical Sciences, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark*

WP 769 **Quantitative analysis and kinetics of Aβ and Tau proteoforms in living human brains**; Reid A Coyle[1]; Soumya Mukherjee[2]; Aram Aslanyan[3]; Yingxin He[2]; Chihiro Sato[2]; Nupur Ghoshal[2]; Junyue Ge[4]; Srinivas Koutarapu[4]; Katherine Schwetye[2]; Kaleigh Roberts[2]; Don Elbert[5]; Jorg Hanrieder[3, 4]; Randall J Bateman[2]; Ross W Paterson[3]; *[1]Washington University St. Louis, St. Louis, MO; [2]Washington University School of Medicine, St. Louis, MO; [3]University College London, London, United Kingdom; [4]University of Gothenburg, Gothenburg, Sweden; [5]University of Washington, Seattle, WA*

WP 770 **The proteome of human and cynomolgus liver**; Yasaman Jami-Alahmadi[1]; Hendrik Neubert[1]; Katherine Wright[1]; Joel Federspiel[1]; Robert Joseph Seward[1]; Pierre M Jean Beltran[2]; *[1]Pfizer Inc., Andover, MA; [2]Pfizer, Inc, Cambridge, MA*

WP 771 **Uncovering the Link Between Chronic Inflammation and Alzheimer's Disease Using Label-Free Mass Spectrometry**; Yijun Chen[1]; Xuemei Zeng[2]; Xinfeng Guo[1]; Xiaohai Wang[1]; Thomas K. Karikari[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Department of Psychiatry, School of Medicine, University of Pittsburgh, Pittsburgh, Pennsylvania*

WP 772 **Deep-coverage Proteomics using a Photocleavable Surfactant Reveals Extracellular Matrix Alterations in Ischemic Cardiomyopathy**; Kevin M Buck[1]; Holden T Rogers[2]; Morgan W. Mann[3]; Timothy Aballo[2]; Zhan Gao[2]; Emily A Chapman[2]; Scott J Price[2]; Ying Ge[2]; *[1]University of Wisconsin-Madison, Madison, WI; [2]UW-MADISON, Madison, WI; [3]Stanford University - Pathology, Stanford, CA*

WP 773 **Single tissue proteomics in Caenorhabditis elegans reveals proteins resident in intestinal lysosome-related**

organelles.; Ting-Yu Wang[1]; Chieh-Hsiang Tan[1]; Heenam Park[1]; Brett Lomenick[1]; Tsui-Fen Chou[1]; Paul W. Sternberg[1]; *[1]California Institute of Technology, Pasadena, CA*

WP 774 **Leveraging the Covaris AFA-sonication to develop a high-throughput assay for deep proteome coverage of fresh frozen tissue sections**; Saeed Seyedmohammad; *Cedars Sinai Medical Institute, Los Angeles, CA*

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WP 775 **Single-Cell Metabolic Fingerprints Discover a Cluster of Circulating Tumor Cells with Distinct Metastatic Potential**; Yun Chen[1]; Feifei Xu[1]; Wenjun Zhang[1]; *[1]Nanjing Medical University, Nanjing, China*

WP 776 **Elemental Analysis in yeast cells and selenium enriched yeast cells by ICP-MS with Automated Micro-Flow Sample Introduction**; Yan Cheung[1]; Emmett Soffey[1]; *[1]Agilent Technologies, Wood Dale, IL*

WP 777 **Expanding the limits of targeted quantitation for low input proteomics using a novel high-speed hybrid nominal mass instrument**; Chris Hsu[1]; Lilian R Heil[2]; Philip M. Remes[2]; Cristina Jacob[2]; Deanna L. Plubell[1]; Bo Wen[3]; Ritin Sharma[4]; Joshua Cantlon[5]; Jesse D. Canterbury[2]; Ping Yip[2]; William Barshop[2]; Vane Shen[2]; Vani Asapu[2]; Claudia Martins[2]; Scott Peterman[2]; Patrick Pirrotte[4]; Mariya T. Sweetwyne[1]; Christine C. Wu[1]; Michael J. MacCoss[1]; *[1]University of Washington, Seattle, WA; [2]Thermo Fisher Scientific, San Jose, CA; [3]University of Washington, Seattle, WA; [4]The Translational Genomics Research Institute, Phoenix, AZ; [5]Scienion, Phoenix, AZ*

WP 778 **Streamlined High-Throughput Single-Cell Proteomics: Tip-Based Sample Preparation for Enhanced Sensitivity and PTM Identification**; Jongmin Woo[1]; Hongyi Liu[1]; Zhenyu Sun[1]; Yuefan Wang[1]; Lijun Chen[1]; Liyuan Jiao[1]; Kay Li[1]; Hui Zhang[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

WP 779 **Investigating cellular diversity through label-free single-cell proteomics**; Qi Wu[1]; Lei Cheng[1]; Robert A. Fenton[1]; *[1]Aarhus University, Aarhus, Denmark*

WP 780 **Exploration of Single Cell Lipidomics with a Novel Multi-reflecting Q-Tof Platform**; Scarlet A Ferrinho[1, 2]; Nyasha Munjoma[2]; Richard Lock[2]; David Heywood[2]; Robert S Plumb[2]; Preeti Mourya[1]; Shazneil Briones[1]; Lee A Gethings[2]; Olivier Cexus[1]; Paul A Townsend[1]; *[1]University of Surrey, Guildford, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom*

WP 781 **Single-cell multi-omics analysis of in vitro post-ovulatory aged oocytes revealed aging-dependent protein degradation**; Xuejiang Guo[1]; Yueshuai Guo[1]; Mengmeng Gao[1]; Xiaofei Liu[1]; Haotian Zhang[1]; Chenghao Situ[1]; Yan Li[1]; *[1]State Key Laboratory of Reproductive Medicine and Offspring Health, Nanjing Medical University, Nanjing, China*

WP 782 **Elevating Single-Cell Proteomics: Maximizing Sensitivity and Throughput with Advanced Chromatographic Separation and MS Data Acquisition Strategies**; Runsheng Zheng[1]; Manuel Matzinger[2]; Rupert Mayer[2]; Tabiwang N Arrey[3]; Alec Valenta[1]; Xufei Sun[4]; Christopher Pynn[1]; Ece Aydin[1]; Wim Decrop[1]; Dominic Hoch[5]; Martin Samonig[1]; Karl Mechtler[2, 6, 7]; *[1]Thermo Fisher Scientific, Germering, Germany; [2]Institute of Molecular Pathology, Campus-Vienna-Biocenter 1, Vienna, Austria; [3]Thermo Fisher Scientific GmbH, Bremen, Germany; [4]Thermo Fisher Scientific, Sunnyvale, CA; [5]Thermo Fisher Scientific, Reinach, Switzerland; [6]Institute of Molecular Biotechnology of the Austrian Academy of Sciences, Vienna, Austria; [7]Gregor Mendel Institute of Molecular Plant Biology of the Austrian Academy of Sciences, Vienna, Austria*

WP 783 **Deep single-cell proteomics of human induced pluripotent stem cells differentiation provides a time-lapse of cell-type specific protein markers**; Pierre Sabatier[1, 2]; Zilu Ye[1, 3]; Maico Lechner[1]; Sergey Rodin[2]; Karl-Henrik Grinnemo[2]; Jesper Velgaard Olsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, Proteomics Program, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; [2]Department of Surgical Sciences, Uppsala University, Uppsala, Sweden; [3]State Key Laboratory of Common Mechanism Research for Major Diseases, Suzhou Institute of Systems Medicine, Suzhou, China*

WP 784 **Single cell Deep Visual Proteomics allows precise spatial mapping of proteomic changes in human liver tissue**; Caroline Weiss[1]; Lauryn Brown[2]; Paolo Pellizoni[3]; Lucas Miranda[3]; Marvin Thielert[1]; Jonathan Hernandez[4]; Karsten Borgwardt[3]; Natalie Porat-Shilom[2]; Florian Rosenberger[1]; Matthias Mann[1]; *[1]Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Thoracic and GI Malignancies Branch, National Cancer Institute, National Institutes of Health, Bethesda, MD; [3]Machine Learning and Systems Biology, Max Planck Institute of Biochemistry, Martinsried, Germany; [4]Surgical Oncology Program, National Cancer Institute, National Institutes of Health, Bethesda, MD*

WP 785 **Phospholipid analysis of single-cells by live single-cell mass spectrometry**; Hajime Mizuno[1]; Aogu Furusho[2]; Jo Sakata[2]; Takuma Yanagisawa[1, 2]; Eiji Sugiyama[2]; Susumu Y. Imanishi[1]; Kenichiro Todoroki[2]; Iwao Sakane[3]; *[1]Meijo University, Nagoya, Japan; [2]University of Shizuoka, Shizuoka, Japan; [3]ITO EN Ltd., Makinohara, Japan*

WP 786 **Single-cell proteomics by mass spectrometry of pre-implantation mouse embryos uncover distinct asymmetry of certain proteins among early blastomeres**; Yuan Yuan[1]; Mo Hu[2]; Yinghui Zheng[1]; Xiaoliang Sunney Xie[1]; *[1]Peking University, Beijing, China; [2]Changping Laboratory, Beijing, China*

WP 787 **Challenging the Astral mass analyzer - going beyond 5200 proteins per single-cell at unseen quantitative accuracy studying cell cycle biology**; Manuel Matzinger[1]; Julia A Bubis[1]; Tabiwang N Arrey[2]; Eugen Damoc[2]; Bernard Delanghe[2]; Karl Mechtler[1]; *[1]Protein Chemistry Group, IMP, Vienna, Austria; [2]Thermo Fisher Scientific, Bremen, Germany*

WP 788 **High throughput single-cell mass spectrometry enabling structural elucidation and relative quantitation of phospholipid C=C isomers**; Chenxi Cao[1]; Simin Cheng[2]; Yao Qian[1]; Zheng Ouyang[1]; Xiaoxiao Ma[1]; *[1]Tsinghua University, Beijing, China; [2]National Institute of Metrology, Beijing, China*

WP 789 **Label-free DIA-based workflow for single-cell proteomic analysis on an Orbitrap Ascend Tribrid mass spectrometer**; Fernanda Salvato[1]; Julia Kraegenbring[2]; Bernard Delanghe[2]; David Hartlmayr[3]; Anjali Seth[3]; Amirmansoor Hakimi[1]; Tonya Pekar Hart[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Cellenion, Lyon, France*

WP 790 **High-throughput Lipidomic Profiling of Individual Mammalian Mitochondria using Image-guided MALDI-2 Mass Spectrometry**; Seth W Croslow[1, 2]; Timothy J Trinklein[1]; Stanislav Rubakhin[1, 2]; Jonathan Sweedler[1, 2]; *[1]Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Champaign, IL; [2]Department of Chemistry, University of Illinois Urbana-Champaign, Champaign, IL*

WP 791 **Going Viral: Sex Heterogeneity of Human Astrocytes' Infection Response through Single-Cell Proteomics**; Shuxin Chi[1]; Arpa Ebrahimi[2]; Jason Rogalski[1]; Claudia Maier[2]; Leonard J Foster[1]; *[1]University of British Columbia, Vancouver, BC; [2]Oregon State University, Corvallis, OR*

WP 792 **Gradient Elution Nanoflow Liquid Chromatography without a Binary Pump: Smoothed Step Gradients Enable Inexpensive, Sensitive and Reproducible Single-Cell Proteomics**; Kei Webber[1]; Siqi Huang[1]; Lavender Lin[1]; Tyler Hunter[1]; Josh Andersen[2]; Ryan T. Kelly[1, 3]; *[1]Brigham Young University, Provo, UT; [2]University of Utah, Salt Lake City, UT; [3]MicrOmics Technologies, Spanish Fork, UT*

WP 793 **High-Throughput Profiling of Lipids and Targeted Proteins Using Microscopy-Guided Single Cell Mass**

Spectrometry; Marisa Asadian[1]; Timothy J Trinklein[1]; Stanislav Rubakhin[1]; Mark J. Lim[2]; Gargey Yagnik[2]; Orly Lazarov[3]; Fan Lam[1]; Kenneth J. Rothschild[2, 4]; Jonathan V. Sweedler[1]; *[1]University of Illinois at Urbana-Champaign, Champaign, Illinois; [2]AmberGen Inc., Billerica, MA; [3]University of Illinois at Chicago, Chicago, IL; [4]Boston University, Department of Physics and Photonics Center, Boston, MA*

WP 794 **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 795 **Single Cell Metabolomics and Proteomics Studies of CRISPR/Cas9 Gene Editing Results**; Tra D Nguyen[1]; Lindsie Martin[1]; Zongkai Peng[1]; Eniola A Adewunmi[2]; Neeraj K Chauhan[2]; Shakya Sankalpani Gunasena Wije Munige[1]; Deepti Bhusal[1]; Rakhi Rajan[1]; Martin-Paul Agbaga[2]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK; [2]The University of Oklahoma Health Sciences Center, Oklahoma City, Oklahoma*

WP 796 **In-depth Proteome Profiling of <1000 bacterial cells**; Andikan Jones Nwosu[1]; Madi Johnston[1]; Cecile Thion[2]; Siqi Huang[3]; Xiaofeng Xie[3]; Ryan T. Kelly[3]; *[1]Brigham Young University, Provo, UT; [2]Cellenion, Lyon, France; [3]Brigham Young University, Provo*

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WP 797 **Analysis of aminated polybutadiene via matrix-assisted laser desorption/ionization - time-of-flight mass spectrometry**; Brennan Curole[1]; Sabrina Scott[2]; Laurel L Schafer[2]; Scott Michael Grayson[1]; *[1]Tulane University, New Orleans, LA; [2]University of British Columbia, Vancouver, BC*

WP 798 **Coupling Multi-Stage Fragmentation with Ion Mobility-Mass Spectrometry for Serial Sequencing of Blocks in Digital Polymers**; Isaure Sergent[1]; Thibault Schutz[2, 3]; Laurence Oswald[3]; Georgette Obeid[2]; Jean-François Lutz[2, 3]; Laurence Charles[1]; *[1]Aix Marseille Université, CNRS, UMR 7273, Institut de Chimie Radicalaire (ICR), Marseille, France; [2]Université de Strasbourg, CNRS, Institut de Science et d'Ingénierie Supramoléculaires (ISIS), Strasbourg, France; [3]Université de Strasbourg, CNRS, Institut Charles Sadron UPR22, Strasbourg, France*

WP 799 **Online Bipolar Dual Spray for the Charge State Reduction and Characterization of Complex Synthetic Polymers**; John Stutzman[1]; Paul D. Hutchins[1]; Ryan M. Bain[1]; *[1]Dow Inc, Midland, MI*

WP 800 **Chemical fingerprinting of synthetic polymers using temperature-programmed direct mass spectrometric analysis**; Ville Nissinen[1]; Krista Gronlund[1]; Mika Suvanto[1]; Jarkko J. Saarinen[1]; Janne Janis[1]; *[1]University of Eastern Finland, Joensuu, Finland*

WP 801 **Identifying Polymers' DART-HRMS Ions for Food Contact Article Screening**; Victoria M Anderson[1]; Jānis Ruško[2]; Ingus Pērkons[2]; Kristen L. Reese[3]; Luke K. Ackerman[3]; *[1]Joint Institute for Food Safety and Applied Nutrition (JIFSAN), University of Maryland, College Park, MD; [2]BIOR Institute of Food Safety, Animal Health and Environment "BIOR", Laboratory of Chemistry, Lejupes street 3, Riga, Latvia; [3]U.S. Food and Drug Administration, Center for Food Safety and Applied Nutrition, 5001 Campus Drive, College Park, MD*

WP 802 **Rapid Characterization of Crosslinked Networks by Thermal Desorption/Pyrolysis Interfaced to Direct Analysis in Real Time Mass Spectrometry (TDPy-DART-MS)**; Calum Bochenek[1]; Tyler C Arntz[1]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH*

WP 803 **Identification of Linear-Dendritic Copolymer Structures via MALDI-TOF MS**; Ashley Miles[1]; Allycea Huskey[1]; Anna Nuzzo[1]; Scott M Grayson[1]; *[1]Tulane University, New Orleans, LA*

WP 804 **Synthesis of Linear and Cyclic Poly(hydroxypivalic acid)**; Amman Nadeem[1]; Lavinia Moon Palmer[1]; Scott Michael Grayson[1]; *[1]Tulane University, New Orleans, LA*

WP 805 **The use of soft ionization in the creation of a searchable pyrolysis GC/MS mass spectral library**; Edward Erisman[1]; Yamil Simón-Manso[1]; William E Wallace[1]; Stephen E Stein[1]; *[1]NIST, Gaithersburg, MD*

WP 806 **Graphical Data Analysis and Sample Comparison of Complex Mesophase Pitches**; Mark A Arnould[1]; Aparna Annamraju[2]; Ercan Cakmak[2]; Frederic Vautard[2]; *[1]Bruker Scientific, LLC, Billerica, MA; [2]Oak Ridge National Laboratory, Oak Ridge, TN*

WP 807 **MALDI-TOF MS Analysis of Mechanopolymers and Vitrimers**; Kushal Modi[1]; Mark A Arnould[1]; Chrys Wesdemiotis[2]; Calum Bochenek[2]; Tyler Arntz[2]; *[1]Bruker Scientific, LLC, Billerica, MA; [2]The University of Akron, Akron, OH*

WP 808 **Investigating the cyclization of linear ethylene brassylate through MALDI-MS**; Mahi Ahmad[1]; Scott Michael Grayson[1]; *[1]Tulane University, New Orleans, LA*

WP 809 **Examination of Self-Healing Thermosets Through Thermal Degradation: Pyrolysis Direct Analysis in Real Time (TDPy-DART-MS) and MALDI Structural Profiling**; Tyler C Arntz[1]; Calum Bochenek[1]; Bryan Katzenmeyer[2]; Robert B Cody[2]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH; [2]JEOL USA, Inc., Peabody, MA*

WP 810 **Deciphering the secrets of environmental polyethylene terephthalates microplastics (PET) by chemical depolymerization and advanced mass spectrometry**; Bayan ALMASRI[1, 2]; Youssef BAKKOUR[2, 3]; Christian ROLANDO[1, 4]; *[1]Miniaturization for Synthesis, Analysis & Proteomics (MSAP), USR 3290, CNRS, University of Lille, Faculty of Sciences & Technologies, Villeneuve d'Ascq, France; [2]Laboratory of Applied Chemistry (LAC), Lebanese University, Faculty of Sciences, Tripoli, Lebanon; [3]King Khalid University, Abha, Saudi Arabia; [4]Shrieking Sixties, 1-3 Allée Lavoisier, Villenueve d'Ascq, France*

TOXICOLOGY
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WP 811 **A Coated Blade Spray Mass Spectrometry Workflow for Rapid Toxicology General Unknown Screening**; David Borts[1]; Laura Burns[1]; Dwayne Schrunk[1]; Shane Stevens[2]; Ryan Micklitsch[2]; *[1]Iowa State University, Ames, IA; [2]Restek Corporation, Bellefonte, PA*

WP 812 **A Triple Quadrupole GC/MS MRM Database for Forensicand Toxicological Workflows**; Celine Gys[1]; Anna Klimowska[1, 2]; Adrian Covaci[1]; Remko Van Loon[3]; Joel Ferrer[4]; Anastasia Andrianova[5]; *[1]Toxicological Center, University of Antwerp, Antwerp, Belgium; [2]Department of Toxicology, Medical University of Gdansk, Gdansk, Poland; [3]Agilent Technologies, Middelburg, Netherlands; [4]Agilent Technologies, Santa Clara, CA; [5]Agilent Technologies, Wilmington, DE*

WP 813 **Rapid Assessment of Toxicants in Emergency Care with Ambient Ionization Mass Spectrometry**; Yi-Wen Hsu[1]; Hung Su[2]; Chi-Wei Lee[1]; Jentaie Shiea[2]; *[1]Institute of Medical Science and Technology, National Sun Yat-sen University, Kaohsiung, Taiwan; [2]Department of Chemistry, National Sun Yat-sen University, Kaoshiung, Taiwan*

WP 814 **Exploring the Toxicity Mechanism of CsPbBr2I Perovskite Quantum Dots by Mass Spectrometry-based Metabolomics**; Cristina Gutierrez Lopez[1]; Gabriel A. Peñalver[1]; Andres Machuca[1]; Estefania Garcia-Calvo[1]; Jose L. Luque-Garcia[1]; *[1]Complutense University of Madrid, Madrid, Spain*

WP 815 **Species-Specific Profiles of Per- and Polyfluoroalkyl Substances in Small Coastal Sharks Along the South Atlantic Bight of the United States**; Qaim Mehdi[1]; Emily K Griffin[1]; Juliette Esplugas[1]; Ashley S Galloway[2]; Bryan S Frazier[3]; Alina S Timshina[1]; R Dean Grubbs[4]; Keyla Correia[1]; Camden G Camacho[1]; Jim Gelsleichter[5]; John Bowden[1]; *[1]University of Florida, Gainesville, FL; [2]South Carolina Department of Natural Resources Marine Resources Division, Charleston, South Carolina; [3]South Carolina Department of Natural Resources Marine Resources Division, Charleston, USA; [4]Florida State University, St.*

Teresa, Florida; [5]University of North Florida, Jacksonville, Florida

WP 816 **Optimized Sample Preparation for Low Level Determination of the Alcohol Marker EtG from Hair Using UPLC-MS/MS Analysis**; Lee Williams[1]; Zainab Khan[1]; Lucy Lund[1]; Adam Senior[1]; Helen Lodder[1]; Russell Parry[1]; Geoff Davies[1]; Alan Edgington[1]; Claire Desbrow[1]; Dan Menasco[1]; Esraa AboJasser[1]; *[1]Biotage GB Limited, Cardiff, United Kingdom*

WP 817 **Evaluating the proteome profiles in juvenile Coho gill and liver tissues exposed to the toxic tire-associated contaminant 6PPD-quinone**; Jason Rogalski[1]; Bonnie P Lo[2]; Xiaojing Yuan[1]; Lok Tin Hui[1]; Vicki L Marlatt[2]; Tanya M Brown[2]; *[1]University of British Columbia, Vancouver, BC; [2]Simon Fraser University, Burnaby, BC*

WP 818 **Untargeted LC-MS/MS Analysis of Drug Metabolites in Human Hepatocyte Suspensions for Comparison to Rat Liver S9 Fractions**; Tyler S. Larson[1]; Krishna Ravindra[2]; Barbara A. Wetmore[3]; Denise K. MacMillan[3]; *[1]Oak Ridge Institute for Science and Education, Oak Ridge, TN; [2]Oak Ridge Associated Universities, Oak Ridge, Tennessee; [3]US Environmental Protection Agency, Research Triangle Park, NC*

WP 819 **Characterization of a Humanized Mouse Model of Organophosphate Poisoning and Detection of Countermeasures via MALDI-MSI**; Caitlin Tressler[1]; Benjamin Wadsworth[2]; Samantha Carriero[2]; Natalie Dillman[1]; Rachel Crawford[1]; C. Linn Cadieux[2]; *[1]Johns Hopkins University, Baltimore, MD; [2]US Army Medical Research Institute for Chemical Defense, Aberdeen Proving Ground, MD*

WP 820 **LC-MS/MS Analysis to Evaluate Hepatotoxicity of Therapeutic Molecules in Cell Media of Complex Liver In Vitro Models**; France Landry[1]; Yongliang (Kevin) Zhang[1]; Vasanthi Bhaskaran[1]; Alexa Murray[2]; Rhiannon Hardwick[2]; Patrick Devine[3]; Petia Shipkova[1]; *[1]Bristol Myers Squibb, Lawrenceville, NJ; [2]Bristol Myers Squibb, San Diego, CA; [3]Bristol Myers Squibb, Cambridge, MA*

WP 821 **Application of High Resolution LC/MS Analysis to In Vitro Comparative Metabolism (IVCM) Samples for the Fungicide Crop Protection Chemical Oxathiapiprolin**; Michael P Mawn[1]; Lingshuang Cai[1]; Vitaly Palamarchouk[1]; Leonid Khyliuk[1]; Jen Goodell[1]; Matthew W Himmelstein[1]; *[1]Corteva Agriscience, Newark, DE*

WP 822 **Rapid high-resolution screening for drugs of abuse with library searching on a novel acoustic ejection HRMS with triple quadrupole confirmation**; Aaron Stella[1]; Jacob McCabe[1]; Anuja Bhalkikar[2]; *[1]SCIEX, USA, Framingham, MA; [2]Sciex, Framingham, MA*

WP 823 **Direct determination of 12 drugs of abuse in saliva using new LDTD Ion Source at 8 seconds per sample**; Jean Lacoursière[1]; Jonathan Rochon[1]; Mégane Moreau[1]; Sarah Demers[1]; Serge Auger[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC*

THURSDAY POSTERS

Set up all Thursday posters
7:00 - 8:00 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
7:00 - 8:00 pm

ANTIBODIES & ANTIBODY DRUG CONJUGATES II
001-033

ThP 001 **Charge variant identification and localization of post-translational modifications with integrated icIEF-UV/MS**; Scott Mack[1]; Jingwen Ding[1]; Zoe Zhang[2]; Maggie Ostrowski[1]; *[1]SCIEX, Fremont, CA; [2]SCIEX, Redwood City, CA*

ThP 002 **Nanoparticle-based enrichment provides deeper insight into host cell proteins in biological drug products**; Samira Vautrin[1]; Emmanuel Nony[2]; *[1]Evotec, München, Germany; [2]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[1]; Scott Berger[1]; Ying Qing Yu[1]; Sean Wu[1]; *[1]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[1]; Ayako Kurimoto[2]; Toshiki Mochizuki[1]; Nana Kasamori[1]; Takafumi Komori[1]; *[1]Eisai Co.,Ltd., Tsukuba, Japan; [2]Protein Metrics, LLC, Cupertino, CA*

ThP 005 **Disulfide Bond Mapping of Cysteine-Engineered Biotherapeutics**; Scott Ugrin[1]; John E Harlan[1]; *[1]AbbVie Inc., North Chicago, IL*

ThP 006 **Charge variant analysis of antibody-drug conjugates using an icIEF-UV/MS approach**; Rashmi Madda[1]; Jingwen Ding[2]; Haichuan Liu[1]; Scott Mack[2]; Maggie Ostrowski[2]; Steven Calciano[2]; Zoe Zhang[1]; *[1]SCIEX, Redwood City, CA; [2]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[1]; Brandon L. Doyle[1]; William D. Holmes[1]; Andrew G. Werner[1]; Andrew W. Carr[1]; Elisabeth Krug[1]; Suzanne E. Stone[1]; *[1]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[1]; Benqian Wei[1]; Joseph Loo[1]; Rachel Loo[1]; *[1]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[1]; Tony Chen[2]; Tao Bo[2]; Tiemin Huang[2]; Min Du[3]; *[1]ThermoFisher Scientific, Shanghai, China; [2]Advanced Electrophoresis Solutions Ltd, Cambridge, ON; [3]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[1]; Gordon Nicol[1]; Ping Jiang[1]; Jie Ding[1]; *[1]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[1]; Xiaoxi Zhang[1]; Min Du[2]; *[1]ThermoFisher Scientific, Shanghai, China; [2]Thermo Fisher Scientific, Lexington, MA*

ThP 012 **Investigation of IgG subclasses with YTE mutation on Stability Properties of monoclonal antibodies**; Koyuki Takenaka[1, 2]; Michael A. Batt[1, 2]; Alexandra M. Miller[2]; Qi G. Zhang[1, 2]; Jeffrey S. Boyles[2]; Joomi Ahn[1, 2]; *[1]Lilly Biotechnology Center, San Diego, CA; [2]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[1]; Siavash Vahidi[1]; *[1]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[1]; Connor Gould[1]; Jill Hochreiter[1]; Qing Ma[1];

Raymond Cha[1]; Robin Difrancesco[1]; Gene D. Morse[1]; Troy D. Wood[1]; *[1]University at Buffalo, Buffalo, NY*

ThP 015 **Discovery and Investigation of G0 Glycan Isomers in an Afucosylated Therapeutic Antibody**; Miyang Li[1]; Sean Shen[1]; Simon Letarte[1]; *[1]Gilead Sciences Inc, Oceanside, CA*

ThP 016 **CE-MS and the Enhanced Charge Variant Analysis in Site-Specific Antibody-Drug Conjugates**; Leo (Lei) Wang[1]; Paul Shen[2]; Larry (Lei) Wang[1]; Christopher Barton[1]; *[1]Takeda, Lexington, MA; [2]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[1]; Marion H. Emmert[2]; Hang Hu[2]; Erik L. Regalado[2]; Rodell C. Barrientos[2]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Merck & Co., Inc., Rahway, NJ*

ThP 018 **HPLC/MS Quantitation of Unconjugated Drugs in the Presence of Antibody Drug Conjugates (ADCs)**; Eric W. Ma[1]; William Mylott[1]; *[1]PPD, Richmond, VA*

ThP 019 **Disulfide Connectivity in Monoclonal Antibodies: Insights from High-Resolution cIMS-MS Analysis**; Hee-Jin Yoo[1]; Duck-Hyun Kim[1]; Abhik Mojumdar[1]; Kun Cho[1]; *[1]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[1]; Manfred Wuhrer[1]; Elena Dominguez-Vega[1]; *[1]Leiden University Medical Center, Leiden, Netherlands*

ThP 021 **Charge variant microheterogeneity explored via icIEF and offline MS analysis of infliximab biosimilars**; Nora Crushell[1]; Anna Mulligan[1, 2]; Sara Carillo[1]; Zarnab Yasmeen[3]; Jean-François Bellec[3]; Jonathan Bones[1, 2]; *[1]The National Institute for Bioprocessing Research & Training, Dublin, Ireland; [2]School of Chemical and Bioprocess Engineering, University College Dublin, Belfield, Ireland; [3]Bio-techne 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[1]; Kristina Wicht[1]; Kevin Roeleveld[1]; *[1]AnaBioTec, Evergem, Belgium*

ThP 023 **Development of a Mildly Denaturing SEC-MS Method for Intact Mass Analysis of Therapeutic Proteins**; Xiaoteng Gong[1]; Song Nie[1]; Timothy-neil Tiambang[1]; Yuetian Yan[1]; Shunhai Wang[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Inc., Tarrytown, NY*

ThP 024 **Digging into Characterizing the Complexity of Charge Heterogeneity of a Novel Antibody Drug Conjugate by icIEF-UV/MS**; Kristen Nields[1]; Hirsh Nanda[2]; Robert Hepler[2]; Mariam S ElNaggar[3]; Scott Mack[3]; Zoe Zhang[3]; *[1]Janssen Biopharmaceticals, Springhouse, PA; [2]Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania; [3]SCIEX, Fremont, CA*

ThP 025 **LC-MS Based Approaches for Determination of Drug-to-Antibody Ratio of an Antibody Drug Conjugate in Human Plasma**; Lucy WR Gao[1]; Xuefei Zhong[1]; Ying Sheng[1]; Yuan Mao[1]; Tao Xing[1]; Yuetian Yan[1]; Shunhai Wang[1]; Ning Li[1]; Albert Torri[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY*

ThP 026 **Top-Down CDR Sequencing of Native Intact mAbs Through Deconvolution of HC+LC Mixture Spectra**; Lily E. Miller[1]; Stephanie Sturgeon[2]; Yury V. Vasilev[2]; Rachel Franklin[2]; Blake Hakkila[2]; Timothy Djang[3]; Alex Gavrilenko[3]; Jhenya Gavrilenko[3]; Panos Iatrou[3]; Stelios Gkegkas[3]; Diana Oppenheimer[2]; Derrill Sturgeon[3]; Joseph Meeuswen[2]; Adrian L Guthals[2]; *[1]University of Oregon, Eugene, OR; [2]Agilent Technologies, Corvallis, Oregon; [3]Devicepros, Boston, USA, MA*

ThP 027 **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[1]; Cynthia Nagy[1]; Jingjing Huang[2]; Christopher Mullen[2]; Graeme C. McAlister[2]; David Bergen[2]; Vlad Zabrouskov[2]; Kristina Srzentić[3]; Kenneth R. Durbin[4]; Rafael Melani[2]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]ThermoFisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Reinach, Switzerland; [4]Proteinaceous, Inc., Evanston, IL*

ThP 028 **Platform-specific Fc N-glycan profiles of an antisperm antibody**; Ellena Nador[1]; Chaoshuang Xia[1]; Philip J. Santangelo[2]; Kevin J. Whaley[3]; Deborah J. Anderson[1]; Catherine E Costello[1]; *[1]Boston University Chobanian & Avedisian School of Medicine, Boston, MA; [2]Emory University, Atlanta, GA; [3]ZabBio, Inc., San Diego, CA*

ThP 029 **LC-MS-based Strategy for Tissue Distribution Analysis of Antibody-Drug Conjugates in Xenograft Mice**; Bo An[1]; Xiaoyu Zhu[1]; Ming Zhang[1]; Jun Qu[1, 2]; *[1]University at Buffalo, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics and Life Sciences, buffalo, New York*

ThP 030 **Studying Fab glycosylated antibody pharmacokinetics in human plasma samples at the subunit level by nano-RP-LC-MS**; Christoph Gstoettner[1]; Manfred Wuhrer[1]; Elena Dominguez Vega[1]; *[1]Leiden University Medical Center, Leiden, Netherlands*

ThP 031 **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[1]; Tahmid Hassan[1]; Ekaterina Deyanova[1]; *[1]Bristol Myers Squibb, Lawrence Township, NJ*

ThP 032 **LC-MS/MS and EndoS2 Workflow for Knock Out Verification of FUT8, the Gene Encoding for α-(1,6) Fucosyltransferase in CHO Cells**; Benjamin Cutak[1]; Amber Petersen[1]; Andrew Feldmann[1]; Andrew Paoletti[1]; Kevin Ray[1]; *[1]MilliporeSigma, Saint Louis, MO*

ThP 033 **Improved characterization of monoclonal antibodies using intact mass analysis and middle-down approaches on a modified Orbitrap Tribrid mass spectrometer**; Jingjing Huang[1]; Christopher Mullen[1]; Kristina Srzentić[2]; Graeme McAlister[1]; Vlad Zabrouskov[1]; Rafael Melani[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Reinach, Switzerland*

ART, ARCHAEOLOGY & PALEONTOLOGY
034-042

ThP 034 **Low-invasive sampling method for taxonomic for the identification of archaeological and paleontological bones by proteomics of their collagens**; Isabelle Fabrizi[1]; Stephanie Flament[1]; Claire Delhon[2]; Lionel Gourichon[2]; Manon Vuillien[2]; Tarek Oueslati[3]; Patrick Auguste[4]; Christian ROLANDO[5]; Fabrice Bray[5]; *[1]MSAP USR 3290, Villeneuve d'Ascq, France; [2]UMR 7264 - CEPAM, Nice, France; [3]UMR8164 – HALMA, Villeneuve d'ascq, France; [4]UMR 8198 - EEP, villeneuve d'ascq, France; [5]MSAP USR 3290, villeneuve d'ascq, France*

ThP 035 **Determination of New Biomarkers in Ceremonial Caffeinated Beverages by High-Resolution Time-of-Flight Mass Spectrometry**; Coley Beavers[1]; Tareq Aziz[1]; Adam King[1]; Susan D Richardson[1]; *[1]University of South Carolina, Columbia, SC*

ThP 036 **Automated high-throughput biological sex identification from dental enamel using targeted proteomics**; Claire Koenig[1]; Patricia Bortel[2]; Ana Martinez-Val[1]; Christopher Gerner[2]; Fabian Kanz[3]; Enrico Cappellini[4]; Jesper Velgaard Olsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research (CPR), University of Copenhagen, Copenhagen, Denmark; [2]Department of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria; [3]Center for Forensic Medicine, Medical University of Vienna, Vienna, Austria; [4]Geogenetics Section, Globe institute, University of Copenhagen, Copenhagen, Denmark*

ThP 037 **Investigating volatilecontaminant mitigation and object cleaning methods via in-situ-SPME sampling**; Erin Birdsall[1, 2]; G. Asher Newsome[1]; Susan Heald[2]; John George[2]; Gwénaëlle Kavich[1]; *[1]Smithsonian Museum Conservation Institute, Suitland, MD; [2]Smithsonian National Museum of the American Indian, Suitland, MD*

ThP 038 **Biological Sex Estimation from Human Dental Enamel using Mass Spectrometry: Test in a Commingled Burial Context from the Iberian Peninsula**; Andrea M Zurek-Ost[1]; Angie L Mordant[1]; Allie Mills[1]; Thomas S Webb[1]; Natalie K Barker[1]; Emma J Bonthorne[2]; Laura Herring[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Aditu Arkeologia, Ubide, Spain*

ThP 039 **Collagen remains in Cretaceous fossil bone from the Isle of Wight (UK) by LC-MS**; Joseph Hubbard[1]; Steven Robinson[2]; Krzystof Pawlak[2]; Stephen Taylor[1]; *[1]University of Liverpool, Liverpool, United Kingdom; [2]Materials Innovation Factory, University of Liverpool, Liverpool, United Kingdom*

ThP 040 **First application of MALDI MSI and machine learning to historic artwork**; Václav Krupička[1, 2]; Florent Grélard[1, 2]; Landry Blanc[1, 2]; Julie Arslanoglu[3]; Aleksandra Popowich[3]; José Luis Lazarte[4]; Nicolas Desbenoit[1, 2]; Caroline Tokarski[1, 2]; *[1]University of Bordeaux, CNRS, Bordeaux INP, CBMN, UMR 5248, Pessac, France; [2]Bordeaux Proteome Platform, University of Bordeaux, Bordeaux, France; [3]Department of Scientific Research, The Metropolitan Museum of Art, New York, NY; [4]Departement of Paintings Conservation, Metropolitan Museum of Art, New York, NY*

ThP 041 **Ancient Animal Diet Determined through Tandem Mass Spectrometry**; George Katselis[1]; Megan ME Tomilin[1]; Paulos Chumala[1]; Tina Greenfield[1]; *[1]University of Saskatchewan, Saskatoon, SK*

ThP 042 **Developing untargeted and targeted proteomics methods for identification of chia oil in viceregal Mexican artworks**; Sarah E. Noll[1]; Aleksandra Popowich[2]; José Luis Lazarte[3]; Catherine Gilbert[4, 5]; Katell Bathany[4, 5]; Caroline Tokarski[4, 5]; Julie Arslanoglu[1]; *[1]Department of Scientific Research, The Metropolitan Museum of Art, New York, NY; [2]Scientific Research Department, The Philadelphia Museum of Art, Philadelphia, PA; [3]Department of Paintings Conservation, The Metropolitan Museum of Art, New York, NY; [4]University of Bordeaux, CNRS, Bordeaux INP, CBMN, UMR 5248, Pessac, France; [5]Bordeaux Proteome Platform, University of Bordeaux, Bordeaux, France*

ARTIFICIAL INTELLIGENCE IN MS INSTRUMENTATION AND APPLICATIONS II
043-070

ThP 043 **Advanced Stochastic Variational Inference for Accurate Constituent Estimation in Nucleic Acid Mixture Models**; Taichi Tomono[1, 2, 3]; Satoshi Hara[1]; Junko Iida[3, 4]; Takashi Washio[1]; *[1]Department of Reasoning for Intelligence, The institute of Scientific and Industrial Research, Osaka University, Ibaraki-shi, Japan; [2]AI Solution Unit, Technology Research Laboratory, Shimadzu Corporation, Soraku-gun, Japan; [3]Shimadzu Analytical Innovation Research Laboratories, Osaka University, Suita-shi, Japan; [4]Life Science Business Department, Analytical & Measuring Instruments Division, Shimadzu Corporation, Kyoto-shi, Japan*

ThP 044 **Zero-shot retention time prediction for unseen post-translational modifications with molecular structure encodings**; Ceder Dens[1]; Darien Yeung[2]; Oleg Krokhin[2]; Kris Laukens[1]; Wout Bittremieux[1]; *[1]University of Antwerp, Antwerp, Belgium; [2]Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB*

ThP 045 **Deep Learning Models for Protein Structure Elucidation from Mass Spectrometry Data**; Steffen Lindert; *The Ohio State University, Columbus, OH*

ThP 046 **Graphormer-IR: Fast and Accurate ML Predictions for Mass Spectrometry-measured IRMPD Spectra**; Cailum MK Stienstra[1]; Liam Hebert[1, 2]; Patrick Thomas[1]; Alexander Haack[1, 3]; W. Scott Hopkins[1, 4, 5]; *[1]University of Waterloo, Waterloo, ON; [2]Cheriton School of Computer Science, Waterloo, ON; [3]Leibniz Universität Hannover, Hannover, Germany; [4]Watermine Innovation, Waterloo, ON; [5]Centre for Eye and Vision Research, Hong Kong, Hong Kong*

ThP 047 **Compression of imaging mass spectrometry datasets using convolutional autoencoders**; Zhongling Liang[1]; Boone M. Prentice[1]; *[1]University of Florida Department of Chemistry, Gainesville, FL*

ThP 048 **UniSpec: Predicting the Full Range of Peptide Fragment Ion Series by Deep Learning Enhances Reliability in Identifying Complex Biological Peptides**; Qian Dong[1]; Xinjian Yan[1]; Joel Lapin[2]; *[1]NIST, Gaithersburg, MD; [2]Georgetown University, Washington Dc, DC*

ThP 049 **Advanced neural network architectures for MS2 spectra encoding**; Joel Lapin[1]; Alfred Nilsson[2]; Lukas Käll[2]; Mathias Wilhelm[1]; *[1]Computational Mass Spectrometry, TUM, Freising, Germany; [2]KTH Royal Institute of Techonology, Stockholm, Sweden*

ThP 050 **iDeepLC: An effective retention time predictor for unseen modified peptides that can differentiate between isomers**; Alireza Nameni[1, 2]; Lennart Martens[2, 3]; Sven Degroeve[1, 2]; Robbin Bouwmeester[2, 3]; *[1]VIB-UGent Center for Medical Biotechnology, Gent, Belgium; [2]Department of Biomolecular Medicine, Ghent University, Gent, Belgium; [3]VIB-UGent Center for Medical Biotechnology, Gent, Belgium*

ThP 051 **Computer Vision-Assisted Robotized Sampling of Volatile Organic Compounds**; Jing-Chi Jang[1]; Pawel L. Urban[1]; *[1]National Tsing Hua University, Hsinchu City, Taiwan*

ThP 052 **Accounting for digestion enzyme bias in the Casanovo de novo peptide sequencing model**; Carlo F Melendez[1]; Justin Sanders[2]; Melih Yilmaz[2]; William S Noble[1]; *[1]University of Washington - Genome Sciences, Seattle, WA; [2]University of Washington, Seattle, WA*

ThP 053 **Accurate prediction of antibody deamidations leveraging high-throughput automated MAM workflow, deep learning, and protein language models**; Ben Niu[1]; Lili Wang[2]; Benjamin Lee[1]; Wen Chen[1]; Henry Chan[1]; *[1]Bristol Myers Squibb, San Diego, CA; [2]University of California, Berkeley, Berkeley, CA*

ThP 054 **Predicting REIMS from MALDI: to prevent destruction of glioblastoma sections used for model improvement**; Thomas Vanhemel[1]; Melanie Nijs[1]; Angeliki Birmpili[2]; Tim Hendriks[2]; Eva Cuypers[2]; Bart De Moor[1]; *[1]KU Leuven, ESAT-STADIUS, Leuven, Belgium; [2]Maastricht University, Maastricht, Netherlands*

ThP 055 **Metabolomics with absolute concentrations but without calibration curves or isotopologues: extension of AI model to instruments not used in training**; Ana S.H. Costa[1]; Bashar Amer[2]; Rahul R. Deshpande[2]; Luke S. Ferro[1]; Jack Howland[1]; Joshua D. Lauterbach[1]; Jefferson G. Pruyne[1]; Devesh Shah[1]; Timothy Kassis[1]; Susan S Bird[2]; Jennifer M Campbell[1]; *[1]Matterworks, Somerville, MA; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 056 **Improved de novo peptide sequencing with higher quality training data**; Melih Yilmaz[1]; William E Fondrie[2]; Wout Bittremieux[3]; Carlo F Melendez[1]; Varun Ananth[1]; Sewoong Oh[1]; William S Noble[1]; *[1]University of Washington, Seattle, WA; [2]Talus Bioscience, Seattle, WA; [3]University of Antwerp, Antwerp, Belgium*

ThP 057 **Enhancing Protein-Based Human Identification Using AI-Extended Mass Spectral Libraries**; Douglas Slotta[1]; Zachary C Goecker[1]; Lewis Y. Geer[1]; *[1]NIST, Gaithersburg, MD*

ThP 058 **LSM1-MS2: A self-supervised foundation model for MS2 downstream tasks including broad chemical property prediction and spectral lookup**; Gabriel Asher[1]; Jennifer M Campbell[1]; Jack Geremia[1]; Timothy Kassis[1]; *[1]Matterworks, Inc., Somerville, MA*

ThP 059 **A Bayesian model for estimating the posterior error probability and the false discovery rate of de novo peptide sequencing**; Ngoc Hieu Tran[1]; Rui Qiao[1]; Lei Xin[1]; Baozhen Shan[1]; *[1]Bioinformatics Solutions Inc, Waterloo, ON*

ThP 060 **Benchmarking machine learning strategies for phosphoproteomic data in clear cell renal carcinoma diagnosis and staging**; Nazrath Nawaz[1]; Weronika E. Borek[1]; Josie A. Christopher[1]; Pedro Moreno-Cardoso[1]; David N. Perkins[1]; Amy E. Campbell[1]; Pedro R. Cutillas[1, 2];

Arran D. Dokal[1]; *[1]Kinomica Ltd, Macclesfield, Cheshire, United Kingdom; [2]Barts Cancer Institute, Queen Mary University of London, London, United Kingdom*

ThP 061 **Breaking Barriers in Complex Sample Analysis: Predicting Total Acid Number and Sulfur Content through FT-ICR-MS Data with Machine Learning Approaches**; Jussara Valente Roque[1]; Wilson Junior Cardoso[2]; Gesiane da Silva Lima[2]; Gabriel Franco Dos Santos[2]; Alexandre de Oliveira Gomes[3]; Iris Medeiros Junior[3]; Boniek Gontijo Vaz[2]; *[1]Universidade Federal de Goiás, Goiânia, Brazil; [2]Universidade Federal de Goias, Goiânia, Brazil; [3]PETROBRAS, Rio de Janeiro, Brazil*

ThP 062 **A learned score function improves the power of mass spectrometry database search**; Varun R Ananth[1]; Justin Sanders[1]; Melih Yilmaz[1]; Sewoong Oh[1]; William S Noble[1, 2]; *[1]Paul G. Allen School of Computer Science and Engineering, University of Washington, Seattle, WA; [2]University of Washington - Genome Sciences, Seattle, WA*

ThP 063 **MassQL Assistant - A Custom GPT4 Assistant To Enhance Accessibility to Query Mass Spectrometry Data with MassQL**; Kartik Gulia[1]; Mingxun Wang[1]; *[1]University of California Riverside, Riverside, CA*

ThP 064 **GraphOmicsNet: an unified pipeline of integrated cancer omics with graph autoencoder for molecular classification of cancers**; Yiyang Chen[1, 2]; Guixue Hou[1, 2]; Siqi Liu[1, 2]; *[1]University of Chinese Academy of Sciences, Beijing, China; [2]BGI, Shenzhen, China*

ThP 065 **Artificially Intelligent copilot for Automating LC-OzESI-MRM Lipidomics Experiments and Analysis using Large Language Models**; Sanjay Iyer[1]; Caitlin E. Randolph[2]; Matthew Muhoberac[2]; Connor Beveridge[2]; Shane Tichy[3]; Gaurav Chopra[2, 4, 5, 6, 7, 8, 9]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, Department of Chemistry, West Lafayette, IN; [3]Agilent Technologies, Santa Clara, CA; [4]Purdue University, Department of Computer Science, West Lafayette, IN; [5]Purdue Institute for Drug Discovery, West Lafayette, IN; [6]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; [7]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; [8]Purdue Institute for Integrative Neuroscience, West Lafayette, IN; [9]Regenstrief Center for Healthcare Engineering, West Lafayette, IN*

ThP 066 **Predicting compositional fragments of compounds from their tandem mass spectra using deep neural networks**; Yuhui Hong[1]; Sujun Li[1, 2]; Yuzhen Ye[1]; Haixu Tang[1]; *[1]Indiana University, Bloomington, IN; [2]GlycoMS LLC, Bloomington, IN*

ThP 067 **Benchmarking prediction models for improved peptide identification with MSBooster and FragPipe**; Kevin L Yang[1]; Fengchao Yu[1]; Ludwig Lautenbacher[2]; Mathias Wilhelm[2]; Alexey I Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, Michigan; [2]Computational Mass Spectrometry, TUM, Freising, Germany*

ThP 068 **Automatic Registration of MALDI images with Atlases**; Pasindu Tennakoon[1]; Pulasthi Ekanayake[1]; Sanoj Silva[1]; Lalin Theverapperuma[1]; Andi Krupke[1]; *[1]Expert Intelligence, Santa Clara, CA*

ThP 069 **Exploring the Future of MS: AI-Guided Design of MALDI Matrices using Theoretical and Empirical Insights**; Carlos A. Padilla[1]; Emmanuel Campo[2]; Luis M. Díaz-Sánchez[1]; Cristian Blanco-Tirado[1]; Aldo F. Combariza[2]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia; [2]Universidad de Sucre, Sincelejo, Colombia*

ThP 070 **Artificially Intelligent copilot for Automating Lipidomics Experiments and Analysis using Large Language Models**; Connor H Beveridge[1]; Matthew Muhoberac[1]; Sanjay Iyer[1]; Caitlin Randolph[1]; Palak Manchanda[1]; Shane Tichy[2]; Gaurav Chopra[3, 4, 5, 6, 7, 8, 9]; *[1]Purdue University Department of Chemistry, West Lafayette, IN; [2]Agilent Technologies, Santa Clara, CA; [3]Purdue University, Department of Chemistry, West Lafayette, IN; [4]Regenstrief Center for Healthcare Engineering, West Lafayette, IN; [5]Purdue Institute for Drug Discovery, West Lafayette, IN; [6]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; [7]Purdue Institute for Integrative Neuroscience, West Lafayette, IN; [8]Purdue University, Department of Computer Science, West Lafayette, IN; [9]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN*

BIOMARKERS: DISCOVERY II
071-100

ThP 071 **EAD-enabled intact glycopeptide/glycoproteome characterization for site-specific glycoproteomics**; Zhengwei Chen[1]; Lei Xiong[2]; *[1]SCIEX, Redwood city, CA; [2]SCIEX, Redwood City, CA*

ThP 072 **Integration of metabolic pathway and network analysis for discovering the biomarkers of fruit-vegetable intervention in pig feces**; Zhihao Liu[1]; Gloria Solano-Aguilar[1]; Sukla Lakshman[1]; Joseph F. Urban[1]; Mengliang Zhang[2]; Pei Chen[1]; Liangli Yu[3]; Jianghao Sun[1]; *[1]USDA-ARS, Beltsivlle, MD; [2]Middle Tennessee State University, Murfreesboro, TN; [3]University of Maryland, College Park, College park, MD*

ThP 073 **Identification of a Lactosylceramide Phosphate as Biomarker for Niemann Pick Disease Type C1**; Sonali Mishra[1]; Pamela Kell[1]; Xuntian Jiang[1]; Dennis J. Dietzen[1]; Charles H. Vite[2]; Elizabeth Berry- Kravis[3]; Stephanie M. Cologna[4]; Forbes D. Porter[5]; *[1]Washington University school of Medicine, St Louis, MO; [2]University of Pennsylvania School of Veterinary Medicine, Pennsylvania, PA; [3]Rush University Medical Center, Chicago, IL; [4]University of Illinois Chicago, Chicago, IL; [5]Arbor Biotechnologies, Cambridge, MA*

ThP 074 **Identification of Biomarkers for Early Detection of Small Cell Lung Cancer Using LC-MS**; Kinnari Chaubal[1]; Yue Li[2]; *[1]Thomas Jefferson High School for Science and Technology, Alexandria, VA; [2]University of Maryland, College Park, College park, MD*

ThP 075 **Decoding Cellular Signatures: Mass Spectrometry Analysis of Exosomes and Total Cellular Proteins from Human Astrocytes and Endothelial Brain Cells**; Kristen H. Hutson[1]; Guoting Qin[2]; Chengzhi Cai[3]; Gergana G. Nestorova[4]; Guoting Qin[2]; *[1]Ph.D. student, Molecular Science and Nanotechnology, Louisiana Tech University, Ruston, LA; [2]Research Associate Professor, College of Optometry, University of Houston, Houston, Texas; [3]Professor, Department of Chemistry, University of Houston, Houston, Texas; [4]Associate Professor, School of Biological Sciences, Louisiana Tech University, Ruston, LA*

ThP 076 **Investigating the Dynamics of the Proteome in the Cerebellum of the Neurodegenerative NPC1 mice model**; Varshasnata Mohanty[1]; Wenping Li[1]; Stephanie M Cologna[1]; *[1]University of Illinois at Chicago, Chicago, IL*

ThP 077 **A Rapid and Economical Workflow to Discover Protein Biomarkers Using High-performance Triple Quadrupole LC/MS System**; Linfeng Wu[1]; Ian Edwards[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 078 **Optimisation of ZenoSWATH DIA workflows for higher throughput plasma protein relative quantification**; Haneen Alharbi[1]; Richard Unwin[1]; *[1]The University of Manchester, Manchester, United Kingdom*

ThP 079 **Reproducibility-optimized multi-group statistic and survival analysis**; Markus Linden[1]; Laura L. Elo[1]; Tomi Suomi[1]; *[1]University of Turku, Turku, Finland*

ThP 080 **Unique high-throughput workflow for deeper plasma/serum proteome coverage enables discovery of novel biomarkers**; Measho Abreha[1]; Katharina Limm[2]; Zehan Hu[2]; Katrin Hartinger[2]; Andreas Schmidt[3]; Sebastian Mueller[4]; Nils A. Kulak[2]; *[1]PreOmics, Billerica, MA; [2]PreOmics, Planegg/Martinsried, Germany; [3]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [4]Biognosys AG, Zuerich, Switzerland*

ThP 081 **Overcoming the dynamic range difficulties in CSF samples through a novel enrichment step for biomarker discovery studies**; Katharina Limm[1]; Zuzana Demianova[1];

Katrin Hartinger[1]; Nils A. Kulak[1]; [1]*PreOmics, Planegg/Martinsried, Germany*

ThP 082 **Deep proteome profiling of Cynomolgus monkey Cerebrospinal Fluid by LCMS**; Xuemei Yang[1]; Youhei Kosugi[1]; Tomoki Yamashita[1]; Faizan Zubair[1]; [1]*Takeda, Cambridge, MA*

ThP 083 **Comparison of Different Collection Methodologies for the Proteomic Analysis of Tear Fluid**; Campbell B Mousseau[1, 2]; Nicole M Schaeublin[1, 2]; Alena R Veigl[1, 2]; Rhonda L Pitsch[2]; Sean W Harshman[2]; [1]*UES, Inc. - an eqlipse company, Dayton, OH;* [2]*Air Force Research Laboratory, Aerospace Systems Directorate, Dayton, OH*

ThP 084 **Identification of Biomarkers in Cerebrospinal Fluid of Schizophrenia Rat Model**; Shideh Mirhadi[1]; Carlo P. Ramil[1]; Mackenzie Hoffmann[2]; Xiaohai Wang[2]; An Chi[1]; [1]*Merck & Co., Inc., Cambridge, MA;* [2]*Merck & Co. Inc., West Point, PA*

ThP 085 **Discovery of metabolite biomarkers of primary headaches with mass spectrometry-based metabolomics**; Shen Hu; *UCLA, Los Angeles, CA*

ThP 086 **Uncovering more biological insights in your samples with routine LC/Q-TOF workflows for metabolites and lipids**; Karen Yannell[1]; Cate Simmermaker[1]; Sierra D. Durham[1]; Genevieve Van De Bittner[1]; [1]*Agilent Technologies, Santa Clara, CA*

ThP 087 **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[1]; Yinghua Yan[1]; [1]*Ningbo University, Ningbo, China*

ThP 088 **Comprehensive TMTpro-16plex based plasma proteome profiling of non-human primate plasma to discover biomarkers for radiation-induced injury**; Mehari Weldemariam[1]; Christina Williams[1]; Maureen A. Kane[1]; [1]*University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, Maryland*

ThP 089 **GlycoISA – Combining Immunosorbent Assay with LC-MS/MS for Glycoproteomic Analysis of Antigen-Specific Antibodies**; Yiyun Liu[1]; Armin Oloumi[1]; Antonio Ji-Xu[1]; Diane Dayoung Park[1]; Ron Feldman[2]; Emanual Maverakis[1]; Carlito B. Lebrilla[1]; [1]*UC Davis, Davis, CA;* [2]*Emory University School of Medicine, Atlanta, GA*

ThP 090 **Dia-PASEF for in-depth immunopeptidomics analysis: Challenges and new opportunities**; Kristina Marx[1]; Naomi Hoenisch Gravel[2, 3, 4]; Torsten Mueller[1]; Pierre-Olivier Schmit[1]; Daniel Hornburg[5]; Juliane Walz[2, 3, 4, 6]; [1]*Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany;* [2]*Department of Peptide-based Immunotherapy, Institute of Immunology, University and University Hospital Tübingen, Tübingen, Germany;* [3]*Cluster of Excellence iFIT (ECX2180) "Image-Guided and Functionally Instructed Tumor Therapies"; University of Tuebingen, Tuebingen, Germany;* [4]*Institute for Cell Biology,Department of Immunology, University of Tuebingen, Tuebingen, Germany;* [5]*Bruker Scientific, 40 Manning Road, Billerica, MA;* [6]*Clinical Collaboration Unit Translational Immunology, Department of Internal Medicine, University Hospital Tuebingen, Tuebingen, Germany*

ThP 091 **Evaluating biofluid biomarker potential of the healthy feline proteome in urine, plasma, and serum**; Katelyn B Brusach[1]; Ariana E Shannon[1]; Brian C Searle[1]; Jessica M Quimby[1]; [1]*The Ohio State University, Columbus, OH*

ThP 092 **Development of red blood cells and plasma-based diagnostic lipid biomarker panel for Parkinson's disease**; Fathima Shaima MuhammedNazaar[1]; Anne M Robets[1]; Ankit Jain[1]; James Doecke[2]; Malcolm Horne[3]; Stephan Klatt[4]; Blaine Roberts[1]; [1]*Emory University, Atlanta, GA;* [2]*CSIRO Health and Biosecurity, Herston, Australia;* [3]*The Florey Institute of Neuroscience and Mental Health, The University of Melbourne, Parkville, Australia;* [4]*Institute for Vascular Signaling, Center for Molecular Medicine, Goethe University, 60590, Germany*

ThP 093 **Proteomic Analysis of Aqueous Humor Biomarkers Associated with Neovascular Complications in Diabetic Retinopathy**; Jaewon Oh[1]; Seong Joon Ahn[2]; Jae Hun Jung[1]; Tae Wan Kim[3]; Kwang Pyo Kim[1]; [1]*Kyung-Hee University, Yong-in, South Korea;* [2]*Hanyang University College of Medicine, Seoul, South Korea;* [3]*SNU, Seoul, South Korea*

ThP 094 **Deciphering Immune Profiles and Proteomic Signatures Correlated with Fusobacterium nucleatum in Colorectal Cancer**; Qiangmin Zhang[1]; Xi Peng[1]; Hyun Young Park[1]; Rosie Blodgett[1]; Patrick Wagner[1]; Kevin (Kunhong) Xiao[1]; [1]*AHN, Pittsburgh, PA*

ThP 095 **Global Proteomics Identifies CDK11 and Spliceosome SF3B1 as Integral to Myeloma Proliferation and High-Risk Disease**; David E Mery[1]; Visanu Wanchai[1]; Timothy Cody Ashby[1]; Samuil Ivanovsky[1]; Hongwei Xu[1]; Eric Siegel[1]; Clyde Bailey[1]; Sandra G Mattox[1]; Samer Al Hadidi[1]; Carolina D Schinke[1]; Sharmilan Thanendrarajan[1]; Maurizio Zangari[1]; Frits Van Rhee[1]; Guido J Tricot[1]; John D Shaughnessy Jr[1]; Fenghuang Zhan[1]; [1]*UAMS, Little Rock, AR*

ThP 096 **Charting the metabolic biogeography of the colorectum in cancer: challenging the proximal versus distal classification**; Abhishek Jain[1]; Caroline Johnson[1]; Sajid A. Khan[2]; Montana T. Morris[2]; Domenica Berardi[1]; Jason Crawford[2]; Noah Palm[2]; Deguang Song[2]; [1]*Yale School of Public Health, New Haven, CT;* [2]*Yale School of Medicine, New Haven, CT*

ThP 097 **Adaptation of plasma-enrichment strategies for fast and sensitive analysis of cerebrospinal fluid**; Eva Borràs[1, 2]; Federica Anastasi[3, 4, 5]; Olga Pastor[1, 2]; Marc Suarez-Calvet[3, 4, 5]; Eduard Sabidó[1, 2]; [1]*Universitat Pompeu Fabra, Barcelona, Spain;* [2]*Centre for Genomic Regulation, Barcelona, Spain;* [3]*BarcelonaBeta Brain Research Center, Barcelona, Spain;* [4]*Pasqual Maragall Foundation, Barcelona, Spain;* [5]*Hospital del Mar Research Institute, Barcelona, Spain*

ThP 098 **Advancing Tear Fluid Proteomics: Optimization of LC-MS/MS Protocol for Enhanced Analysis**; James Xiao[1]; Sally Fu[1]; Kyla Frenia[1]; Jackie Sikora[1]; Leanne Labriola[1]; [1]*Innsight Technology, INC., Pittsburgh, PA*

ThP 099 **Alterations in tear proteomes of adults with pre-diabetes and type 2 diabetes mellitus but without diabetic retinopathy**; Guoting Qin[1, 2]; Cecilia Chao[1, 2]; Shara Duong[1]; Jennyffer Smith[1]; Hong Lin[3]; Jennifer Copeland[4]; Huamin Cai[4]; Stan Stearns[4]; Kathryn Richdale[1]; Wendy Harrison[1]; Chengzhi Cai[1]; [1]*University of Houston, Houston, TX;* [2]*University of New South Wales, Sydney, Australia;* [3]*University of Houston-Downtown, Houston, TX;* [4]*VICI Valco Instruments, Houston, TX*

ThP 100 **Proteome Analysis of Isolated Exosomes from Control and Toxicant-Exposed Bronchoalveolar Lavage Fluids**; Zachary Hutchins[1]; Yinsheng Wang[2]; Andrea Adamcakova-Dodd[3]; Abu Eabrahim Siddique[3]; [1]*University of California, Riverside, Redlands, CA;* [2]*University of California, Riverside, Riverside, CA;* [3]*University of Iowa, Iowa City, IA*

BIOMARKERS: QUANTITATIVE ANALYSIS III
101-127

ThP 101 **Validated Biomarker Assay for the Analysis of Coproporphyrin I and Coproporphyrin III in Human Plasma**; Shane Karnik[1]; John Begley[1]; Benjamin Begley[1]; Davonne J Auguste[1]; Mathew Begley[1]; [1]*Aliri Bioanalysis, COLORADO SPGS, CO*

ThP 102 **Comparative Analysis of Skyline and SmartPeak Performance in Quantifying a 60-Biomarker Panel in Plasma from Inflammatory Bowel Disease Patients**; Dragana Noe[1]; Chi D. L. Nguyen[1]; Erika Hernandez[1]; Jonathan T. Bui[1]; Jennifer E. Van Eyk[2]; Susan M. Mockus[1]; [1]*Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA;* [2]*Advanced Clinical BioSystems Research Institute, Cedars-Sinai Medical Center, Los Angeles, CA*

ThP 103 **LC-MS/MS Method Development of Endogenous Small Molecule Biomarker: Case Studies**; Jingguo Hou[1]; Xiaodong Zhu[1]; Sarah Garcia[1]; Steven Hoehne[1]; Xiaomei Bian[1]; Leimin Fan[1]; [1]*Worldwide Clinical Trials, Austin, TX*

ThP 104 **A Fully Validated Automated Method for the Detection of Cotinine and Hydroxycotinine in Human Serum: Hamilton Vantage™ and LC/MS/MS**; Danielle L Sowle[1]; Tiffany Seyler[1]; Madeline Weaver[2]; Lanqing Wang[1]; *[1]CDC, Atlanta, GA; [2]Oak Ridge Institute for Science and Education, Oak Ridge, TN*

ThP 105 **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[1, 2]; Chao Xue[1, 2]; Xiaoyu Zhu[1, 2]; Jun Qu[1, 2]; *[1]University at Buffalo, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics and Life Sciences, buffalo, New York*

ThP 106 **Quantification of plakophilin 2A in human heart by high resolution mass spectrometry**; Kevin P. Gillespie[1]; Clementina Mesaros[1]; Ian Alexander Blair[1]; *[1]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*

ThP 107 **Integrated Assay Development Platform for in vivo Target Detection in Support of Drug Discovery**; Jingjing Deng[1]; Bogdan Sleczka[1]; Josh Nicklay[1]; Eugene Ciccimaro[1]; Petia Shipkova[1]; *[1]BMS, Princeton, NJ*

ThP 108 **Facilitating precision medicine through targeted proteomics analysis of dried plasma from fingerpricks**; Andreas Hober[1]; Marcus Henricsson[1]; Remco Van Soest[2]; Sahana Mollah[2]; Patrick Pribil[3]; Tasso Miliotis[1]; *[1]AstraZeneca, Mölndal, Sweden; [2]SCIEX, Redwood City, CA; [3]SCIEX, Concord, ON*

ThP 109 **Unveiling Hidden Depths: A High-Throughput Plasma Proteomics Workflow for Enhanced Biomarker Discovery on Orbitrap Astral Mass Spectrometer**; Kevin Yang[1]; Nicholas Mucci[2]; Evangelina Bahu[2]; Andrea Cerda[2]; Lee Cantrell[2]; Khatereh Motamedchaboki[1]; Stephanie Samra[1]; Amirmansoor Hakimi[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Seer Inc., Redwood City, CA*

ThP 110 **Development of Isobaric Peptide Probes for Multiplex Disease Detection using Mass Spectrometry-Based Immunoassay**; Stephanee Joy B Zerrudo[1]; Ayesha Seth[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

ThP 111 **Know Your Proteome: Exploring personalized proteomics in precision health**; Felicia K Ooi[1]; Monica Ghaly[1]; Santosh D Bhosale[1]; Stephen A. Whelan[1]; Susan M Mockus[1]; *[1]Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA*

ThP 112 **Development and Optimization of a LC-MS/MS Method for Accurate Quantification of NAD+ and NAADP Dinucleotides**; Elias Beretta[1]; Yongjin Yao[1]; Danielle Tonev[1]; Purvi Jejurkar[1]; *[1]AbbVie, South San Francisco, CA*

ThP 113 **Low-pg/mL quantitation of leucine-rich repeat kinase 2 (LRRK2) using LC-MS/MS in human cerebrospinal fluid (CSF)**; Jason Causon[1]; Dylan Bennett[2]; Arash Rassoulpour[2]; Rahul Baghla[3]; *[1]SCIEX, Framingham; [2]Neuron23, South San Francisco, CA; [3]SCIEX, Redwood City, CA*

ThP 114 **A CLIA Accredited, GCP-Compliant, high-throughput LC-MS/MS Method for Quantification of Phenylalanine and Tyrosine in Human K2EDTA Plasma**; Nicole Boone[1]; Tian-Sheng Lu[1]; Shuyu Hou[1]; *[1]Medpace, Cincinnati, OH*

ThP 115 **The combination of pharmacokinetic studies and targeted metabolomics as a powerful tool for identifying exposure biomarkers of apple intake**; Shengmin Sang[1]; Junhe Yu[1]; Weixin Wang[1]; Yingdong Zhu[1]; *[1]North Carolina A&T State University, Kannapolis, NC*

ThP 116 **Development of highly sensitive mass spectrometry methods for phosphorylated protein analysis**; Siqi Li[1]; Wayne Leifert[2, 3]; Tara Pukala[1]; *[1]Univerisity of Adelaide, School of Physics, Chemistry and Earth Sciences, Adelaide, Australia; [2]University of Adelaide, School of Biological Sciences, Adelaide, Australia; [3]CSIRO Health and Biosecurity, Adelaide, Australia*

ThP 117 **An LC-MS/MS Method for Detection of a Panel of Steroids Related to The Hypertension for In Vivo Samples**; Hongfang Cui[1]; Hongmei Wang[1]; Hefeng Zhang[1]; Zhiren Yu[1]; Nan Zhao[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

ThP 118 **An LC-MS/MS method for the determination of tetrodotoxin (TTX) in SLC transporters**; Lingyan Hua[1]; Dan Li[1]; Yangzhen Zheng[1]; Jinlian Lu[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

ThP 119 **PRM method development for lung cancer patient classification integrated into a clinical decision support system, the Molecular Tumor Board Portal**; Georgios Mermelekas[1]; Olena Berkovska[1]; David Tamborero[1]; Lukas Orre[1]; Janne Lehtio[1]; *[1]Karolinska Institutet, Solna, Sweden*

ThP 120 **Proteoverse™; an easy-accessible and interactive web interface to help users generate insights into their proteomics data**; Patrick Vanzalm; *Biognosys, Zurich, Switzerland*

ThP 121 **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[1]; Jenn Morris[1]; Kenesha Riley[1]; Clare Hoover[2]; Deborah Berry[1]; David Chain[1]; Yeoun Jin Kim[1]; *[1]AstraZeneca, Gaithersburg, MD; [2]AstraZeneca, Waltham, MA*

ThP 122 **Identification and quantification of phospholipids in contact lens deposits**; Mengyu Xu[1]; Fang Lu[1]; *[1]Johnson & Johnson Vision, Jacksonville, Florida*

ThP 123 **Empowering Translational Research: High-Throughput Plasma Proteomics for Precision Medicine on Orbitrap Exploris 480 Mass Spectrometer**; Kevin Yang[1]; Nicholas Mucci[2]; Evangelina Bahu[2]; Andrea Cerda[2]; Lee Cantrell[2]; Khatereh Motamedchaboki[1]; Stephanie Samra[1]; Amirmansoor Hakimi[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Seer Inc., Redwood City, CA*

ThP 124 **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[1]; Anna Chen Guttman[1]; John-Paul Oliveria[1]; William Rodney Mathews[1]; Michele A. Grimbaldeston[1]; Veronica Anania[1]; *[1]Genentech Inc, South San Francisco, CA*

ThP 125 **Multi-OMICS biosignature phenotype stratification analysis for monitoring personal health optimization**; Stephen A. Whelan[1]; Felicia K Ooi[1]; Nathan Hendricks[1]; Dragana Noe[1]; Susan M. Mockus[1]; *[1]Cedars-Sinai Precision Biomarker Labs (PBL), Beverly Hills, CA*

ThP 126 **A Sensitive and Simple LC-MS/MS Method for Simultaneous Determination of GABA and GHB in Plasma**; Haiyan Li[1]; Cheng Chen[1]; Meijuan He[1]; Xinxin Wen[1]; Xiaotong Li[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

ThP 127 **Liquid Chromatography and Tandem Mass Spectrometry for Quantitation of Endogenous Enantiomers of 3-Hydroxybutyric Acid in Dog Plasma**; Na Li[1]; Li Gao[1]; Yanfu Ren[1]; Zhiyu Li[2]; Lili Xing[2]; Yi Tao[2]; Liang Shen[2]; *[1]WuXi AppTec, Suzhou, China; [2]WuXi AppTec, Shanghai, China*

CANCER RESEARCH II
128-161

ThP 128 **Mass spectrometry-based analysis of proteins and intact glycopeptides in patient urine samples reveals differences associated with prostate cancer**; Nikhiya Shamsher[1]; Fernando Garcia-Marques[1]; Abel Bermudez[1]; Mark R Flory[2]; Sharon J Pitteri[1]; *[1]Canary Center at Stanford for Cancer Early Detection, Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; [2]Cancer Early Detection Advanced Research (CEDAR) Center, Knight Cancer Institute, Oregon Health & Science University, Portland, OR*

ThP 129 **NanoLC-MS/MS DIA Unveils Unfolded-Protein-Response Landscape in Glioma: Illuminating PERK Branch Influence on Lysosomal Dynamics and Ganglioside Fluctuation**; Alexander Wenger[1]; Emma Phillips[2]; Chi D. L. Nguyen[3]; Violaine Rosenstiel-Goidts[2]; Robert Ahrends[1, 3]; *[1]University of Vienna / Department of Chemistry / Institute of Analytical Chemistry, Vienna, Austria;*

[2]DKFZ German Cancer Research Center, Heidelberg, Germany; [3]Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., Dortmund, Germany

ThP 130 **Distinct Plasma Molecular Profiles Between Early-onset and Late-onset Colorectal Cancer Patients Revealed by Metabolic and Lipidomic Analyses**; Shiqi Zhang[1]; Rui Xu[1]; Ming Hu[1]; Fouad Choueiry[1]; Ning Jin[1]; Jieli Li[1]; Xiaokui Mo[1]; Jiangjiang Zhu[1]; *[1]The Ohio State University, Columbus, OH*

ThP 131 **Quantitative Profiling of On-tissue Lipids During Medulloblastoma Metastasis via Aziridination-based Isobaric Mass Tag Labeling and Isomer-resolved Mass Spectrometry Imaging**; Jiaxin Feng[1]; Zilu Huang[2, 3]; Dallas Freitas[4]; Tingyuan Yang[4]; Xi Chen[4]; Shuli Tang[4]; Yuhan Yang[5]; Yun Huang[5]; Yuchen Du[2, 3]; Xiaonan Li[2, 3]; Xin Yan[4]; *[1]TAMU, College Station, TX; [2]Ann & Robert H. Lurie Children's Hospital of Chicago, Chicago, IL; [3]Robert H. Lurie Comprehensive Cancer Center, Feinberg School of Medicine, Northwestern University, Chicago, IL; [4]Texas A&M, College Station, TX; [5]Center for Epigenetics & Disease Prevention, Texas A&M Institute of Biosciences and Technology, Houston, TX*

ThP 132 **DESI-MSI Reveals Insights into Metabolic Alterations Associated with Resistance to Immune Checkpoint Inhibitors in Triple Negative Breast Cancer**; Keziah E Liebenberg[1]; Liqun Yu[1]; Meredith L Spradlin[1]; Xiang Zhang[1]; Livia S Eberlin[1]; *[1]Baylor College of Medicine, Houston, TX*

ThP 133 **Prostate Cancer Reshapes the Secreted and Extracellular Vesicle Urinary Proteomes**; Amanda Khoo[1]; Meinusha Govindarajan[1]; Zhuyu Qiu[2]; Lydia Y. Liu[1]; Vladimir Ignatchenko[1]; Matthew Waas[1]; Andrew Macklin[1]; Alexander Keszei[1]; Brian P. Main[3]; Lifang Yang[3]; Raymond S. Lance[4]; Michelle R. Downes[5]; O. John Semmes[3]; Danny Vesprini[5]; Stanley Liu[5]; Julius O. Nyalwidhe[3]; Paul C. Boutros[2]; Thomas Kislinger[1]; *[1]Princess Margaret Cancer Centre, Toronto, ON; [2]UCLA, Los Angeles, CA; [3]Eastern Virginia Medical School, Norfolk, VA; [4]Spokane Urology, Spokane, WA; [5]Sunnybrook Health Sciences Centre, Toronto, ON*

ThP 134 **A robust metabolic biomarker signature of FASN inhibition**; Dzmitry Mukha[1]; Jena Dessain[1]; Seamus O'Connor[1]; Katherine Pniewski[1]; Fabrizio Bertolazzi[1, 2]; Jeet Patel[3]; Mary Mullins[3]; Zachary Schug[1]; *[1]The Wistar Institute, Philadelphia, PA; [2]Cellular and Molecular Biology Program, Department of Pharmacy and Biotechnology, University of Bologna, Bologna, Italy; [3]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*

ThP 135 **Heterogeneity of drug responses across various lung cancer cell lines with differing genetic backgrounds**; CHUWEI LIN[1]; Devin Schweppe[1]; Katarina Vlajic[1]; Catherine Sniezek[1]; *[1]University of Washington - Genome Sciences, Seattle, WA*

ThP 136 **The proteome and post-translational modification landscape of 54humancancer cell lines - a resource for biomedical studies**; Wenhao Shi[1]; Tianlong He[2]; Nan Wang[3]; Shaojun Tang[2]; Yiying Zhu[4]; *[1]Tsinghua University, Beijing, China; [2]The Hong Kong University of Science and Technology, Hong Kong, Hong Kong; [3]Fynn Biotechnology, Jinan, China; [4]Tsinghua Univeristy, Beijing, China*

ThP 137 **Trapped Ion Mobility Spectrometry (TIMS) enables Deep Coverage of Ras-family members of small GTPases**; Tobias M Maile[1]; Hendry S Cahaya-Healey[1]; Dina J Ghandour[1]; Paul D Schnier[1]; *[1]Loxo@Lilly, South San Francisco, CA*

ThP 138 **Proteogenomic biomarkers of recurrence after curative-intent surgery of colorectal liver metastases**; Geoffrey Y.M. Wong[1, 2]; Jun Li[2, 3]; Matthew J McKay[2, 3]; Nazim Bhimani[1]; Connie Diakos[4, 5]; Thomas J Hugh[1, 5]; Mark P Molloy[2, 3]; *[1]Department of Upper Gastrointestinal Surgery, Royal North Shore Hospital, Sydney, Australia; [2]Bowel Cancer and Biomarker Laboratory, The University of Sydney, Sydney, Australia; [3]Kolling Institute, Royal North Shore Hospital, Sydney, Australia; [4]Department of Medical Oncology, Royal North Shore Hospital, Sydney, Australia; [5]Northern Clinical School, The University of Sydney, Sydney, Australia*

ThP 139 **Revealing the Phosphorylation and Structural Complexity of Neurofibromin**; Robert A. D'Ippolito[1]; Jennifer Mehalko[1]; Pedro Diaz-Parga[1]; Matthew R. Drew[1]; Scott Eury[1]; Katie Powell[1]; Grace M. Scheidemantle[1]; Vanessa Wall[1]; William Burgan[1]; Dominic Esposito[1]; Frank McCormick[1, 2]; Dwight V. Nissley[1]; Caroline J. DeHart[1]; *[1]Frederick National Laboratory for Cancer Research, Frederick, MD; [2]Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA*

ThP 140 **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[1]; Tommy Shields[1]; Vinothini Rajeeve[1]; Pedro Rodriguez Cutillas[1]; *[1]Barts Cancer Institute, Queen Mary University of London, London, United Kingdom*

ThP 141 **Characterizing the role of EED and SUZ12 in the epigenetic reprogramming of MPNST**; Joanna K Lempiainen[1]; Kirill Miachin[1]; Yixuan Axe Xie[1]; Xingyu Liu[1]; Emily Zahn[1]; Kuangying Yang[2]; Angela C Hirbe[2]; Benjamin A Garcia[1]; *[1]Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, St. Louis, MO; [2]Division of Oncology, Washington University School of Medicine, St. Louis, MO*

ThP 142 **Cell-type resolved spatial proteogenomics on human FFPE cancer tissue to characterize molecular trajectories in melanoma progression**; Maximilian Zwiebel[1]; Thierry M. Nordmann[1]; Katrin Kerl-French[2]; Rudolf Stadler[3]; Reinhard Dummer[4]; Matthias Mann[1, 5]; *[1]Department of Proteomics and signal Transduction, Max-Planck-Institute of Biochemistry, Martinsried (near Munich), Germany; [2]Department of Dermatology and Allergology, Ludwig Maximilian University of Munich, Munich, Germany; [3]Department of Dermatopathology, Johannes Wesling Klinikum Minden, Ruhr University Bochum, Minden, Germany; [4]Department of Dermatology, University Hospital Zurich, Zurich, Switzerland; [5]Novo Nordisk Foundation Center for Protein Research (CPR), University of Copenhagen, Copenhagen, Denmark*

ThP 143 **Proteomic Exploration Unveiling the Role of SAP25 in Sin3-Mediated Transcriptional Repression**; Pratik Goswami[1]; Charles A S Banks[2]; Janet Thornton[1]; Bethany Bengs[3]; Mihaela E. Sardiu[3, 4]; Laurence Florens[2]; Michael P Washburn[1]; *[1]Department of Cancer Biology, University of Kansas Medical Center, Kansas City, Kansas 66160; [2]Stowers Institute for Medical Research, Kansas City, Missouri 64110; [3]Department of Biostatistics & Data Science, University of Kansas Medical Center, Kansas City, Kansas; [4]University of Kansas Cancer Center, Kansas City, Kansas*

ThP 144 **Picosecond Infrared Laser Mass Spectrometry enables non-subjective diagnosis of spinal cancers, addressing the high discordance rate in standard of care**; Alexa N Fiorante[1]; Michael Woolman[1]; David Munoz[1]; Gelareh Zadeh[1]; Sunit Das[1]; Howard Ginsberg[1]; Arash Zarrine-Afsar[1]; *[1]University of Toronto, Toronto, ON*

ThP 145 **Deep Quantitative Proteomics Identifies Conserved Proteome Alterations in Low and High-Grade Serous Ovarian Cancers**; Jonathan Ogata[1]; Christopher Tarney[1]; Paulette Mhawech-Fauceglia[1]; Julie Oliver[1]; Tamara Abulez[1]; Brian Hood[1]; Kelly Conrads[1]; Kendal Rosalik[2]; Kwong-Kwok Wong[3]; David Gershenson[3]; Sanghoon Lee[3]; Anil Sood[3]; Kathleen Darcy[1]; Neil Phippen[1]; G. Larry Maxwell[1]; Thomas Conrads[1]; Nicholas W. Bateman[1]; *[1]Women's Health Integrated Research Center, Annandale, VA; [2]Department of Gynecologic Surgery and Obstetrics, Madigan Army Medical Center,, Joint Base Lewis-McChord, WA; [3]Department of Gynecologic Oncology and Reproductive Medicine, The University of Texas MD Anderson Cancer Center, Houston, TX*

ThP 146 **Understanding Drug Resistance Mechanisms in Lung Cancer: Insights from Proteomic Analysis of ABCB1 Overexpression in A549 Cells**; Geul Bang[1]; Ye Eun Park[2];

Eun Hee Han[2]; Jin Young Kim[2]; *[1]Korea Basic Science Institute, Cheongju, South Korea; [2]Korea Basic Science Institute, Cheongju, South Korea*

ThP 147 **Detection of pancreatic cancer cells using aptamers**; Anna Drabik[1]; Joanna Ner-Kluza[1]; Marek Sierzega[2]; *[1]AGH University, Krakow, Poland; [2]Department of General, Oncological and Gastrointestinal Surgery, Jagiellonian University Medical College, Krakow, Poland, Krakow, Poland*

ThP 148 **Development of a High-Throughput LC-MS/MS Assay for A-to-I RNA Editing Analysis by ADAR1 in Cancer Drug Discovery**; Timothy He[1]; Jessica MacManus[1]; Lilu Guo[1]; Bailin Zhang[1]; *[1]Sanofi, Cambridge, MA*

ThP 149 **Characterizing metabolomic heterogeneity in human breast tumour-derived subclonal populations**; Brandon Y. Lieng[1]; William D. Gwynne[1]; Mathula Muhundan[1]; Alexandra J. Denhart[1]; Andrew T. Quaile[1]; Jeremy K. Chan[1]; Nicholas S. Ly[1]; J. Rafael Montenegro-Burke[1]; *[1]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON*

ThP 150 **Analyzing Senolytic Compounds induced Cellular Senescence Response using a Triple Quadrupole Mass Spectrometer**; Evelyn H. Wang[1]; Stephen Kurzyniec[1]; Yoshiyuki Okamura[1]; Yang Yang[2]; Dongwen Lyu[2]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]University of Texas Health Science Center at San Antonio, San Antonio, TX*

ThP 151 **Metabolomic Technologies in the bedside diagnosis and treatment of precancerous cervical disease**; Apostolia Galani[1]; Maria Paraskevaidi[1]; Stefania Maneta-Stavrakaki[1]; Daniel Simon[1]; Jinshi Zhao[1]; Burak Temelkuran[1]; Deidre Lyons[1]; Zoltan Takats[1]; Maria Kyrgiou[1]; *[1]Imperial College London, London, United Kingdom*

ThP 152 **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[1]; Becki Dudley[2]; Matthew Glover[1]; Desmond Jones[2]; Sonja Hess[1]; *[1]AstraZeneca, Gaithersburg, MD; [2]AstraZeneca, Cambridge, United Kingdom*

ThP 153 **Detections of metabolic activity in human glioblastoma cell lines with U-13C glucose by LC-HR-MS with targeted and untargeted analysis**; Erik Peterson[1]; Liddy McCulla[1]; Li Zhang[1]; Xiaoyi Li[1]; Mack Reynolds[2]; Shivam Panda[1]; Hammad Khan[1]; Harrison Wong[1]; Peter Sajjakulnukit[1]; Costas A Lyssiotis[1]; Daniel Wahl[1]; *[1]University of Michigan, Medical School, Ann Arbor, Michigan; [2]University of Michigan, Immunology Program, Ann Arbor, MI*

ThP 154 **Comprehensive Proteogenomic Analysis of Renal Cell Carcinoma Reveals Distinct Molecular Profiles**; Hongyi Liu[1]; Lijun Chen[1]; Yuefan Wang[1]; T. Mamie Lih[1]; Yingwei Hu[1]; Hui Zhang[1]; Clinical Proteomic Tumor Analysis Consortium[2]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD; [2]NIH, Bethesda, MD*

ThP 155 **The proteomic landscape of exhaustion in antigen-specific T cells**; Christian M Beusch[1]; Abdelhameed Dawood[1]; Sarah Welbourn[1]; Ahmet Ozdilek[1]; Mohamed Hakeem[1]; David Gordon[1]; *[1]Emory University School of Medicine, Atlanta, GA*

ThP 156 **Cell-type resolved proteomics identifies and quantifies Merkel Cell Polyomavirus proteins directly in Merkel Cell Carcinoma tissue**; Andreas Metousis[1]; Tim Heymann[1]; Lisa Schweizer[1]; Pia-Charlotte Stadler[1, 2]; Rudolf Stadler[3]; Thierry M. Nordmann[1]; Matthias Mann[1]; *[1]Department of Proteomics and Signal Transduction, Max-Planck-Institute of Biochemistry, Martinsried, Germany; [2]Department of Dermatology and Allergology, Ludwig Maximilian University of Munich, Munich, Germany; [3]University Department for Dermatology, Venereology, Allergology and Phlebology, Skin Cancer Center Johannes Wesling Medical Center, Ruhr University Bochum, Minden, Germany*

ThP 157 **Investigating the Role of mSWI-SNF in the Pathogenesis of Malignant Peripheral Nerve Sheath Tumors**; Kirill Miachin[1]; Joanna K Lempiainen[2]; Yixuan Axe Xie[2]; Angela C Hirbe[3]; Benjamin A Garcia[2]; *[1]Washington University in Saint Louis, St. Louis, MO; [2]Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, St. Louis, MO; [3]Division of Oncology, Washington University School of Medicine, St. Louis, MO*

ThP 158 **Comparison of LIRADS 5 Image Guided Biopsies From FFPE and Frozen Cores for Radiogenomics and Radioproteomics in Different HCC grades**; Margaret Simonian[1]; David SK Lu[1]; Julian Whitelegge[1]; Whitaker Cohn[1]; Preeti Ahuja[1]; William Hsu[1]; Steven S Raman[1]; *[1]UCLA, Los Angeles*

ThP 159 **The distinction of mouse breast cancer by cholesterol profile using ToF-SIMS**; Auraya Manaprasertsak[1]; Per Malmberg[2]; Emma Hammarlund[1]; *[1]Lund University, Lund, Sweden; [2]Chalmers University of Technology, Gothenburg, Sweden*

ThP 160 **Unraveling the Mechanism of Cisplatin Resistance in TNBC: Insights from Metabolomic Profiling via Mass Spectrometry Analysis**; Shashwati Parihari[1]; Anvita Pant[2]; Sanjeeva Srivastava[1]; *[1]IIT Bombay, Mumbai, India; [2]University of Lausanne, Lausanne, Switzerland*

ThP 161 **Isolation of plasma-derived extracellular vesicles using the Mag-Net method to identify potential protein signatures for diagnosis of pancreatic ductal adenocarcinoma**; Sindisiwe Gamelihle Buthelezi[1]; Ireshyn S Govender[1, 2]; Previn Naicker[1]; Andrea Ellero[2, 3]; Stoyan Stoychev[2]; Nnenna Elebo[4]; Jones Omoshoro-Jones[4]; John Devar[4]; Martin Smith[4]; Ekene Emmanuel Nweke[4]; *[1]Council for Scientific and Industrial research, Pretoria, South Africa; [2]ReSyn Biosciences, Pretoria, South Africa; [3]University of Pretoria, Pretoria, South Africa; [4]University of the Witwatersrand, Johannesburg, South Africa*

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ThP 162 **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[1]; Nicholas E Manicke[1]; Lindsey Kirkpatrick[1, 2]; *[1]IUPUI, Indianapolis, IN; [2]Riley Hospital for Children at Indiana University Health, Indianapolis, Indiana*

ThP 163 **Multidimensional Mass Profiles Increase Confidence in Bacterial Identification When Using Low-Resolution Mass Spectrometers**; Zachary J. Sasiene[1]; Erick S. LeBrun[1]; Nileena Velappan[1]; Austin R. Anderson[1]; Nathan H. Patterson[2]; Martin Dufresne[2]; Melissa A. Farrow[2]; Emilio S. Rivera[1]; Lauren K. Heine[1]; Chi-Yen Tseng[1]; Jessica A. Salgueiro[1]; Salvator J. Palmisano[1]; Francisca E. Rodriguez[1]; Tara Harvey[1]; Abigale S. Mikolitis[1]; Kes A. Luchini[1]; Grace M. Thornhill[1]; Brett R. Blackwell[1]; Joshua D. Breidenbach[1]; Phillip M. Mach[1]; Jeremy L. Norris[2]; Richard M. Caprioli[2, 3, 4, 5]; Ethan M. McBride[1]; Trevor G. Glaros[1]; *[1]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Chemistry, Vanderbilt University, Nashville, TN; [5]Department of Pharmacology, Vanderbilt University, Nashville, TN*

ThP 164 **Proteomics profiling for invasive apocrine breast carcinoma provides subclassification, disease mechanisms and guidance on the administration of chemotherapy**; Yiying Zhu[1]; Mengping Long[2]; Wenhao Shi[1]; Tianlong He[3]; Taobo Hu[2]; Shaojun Tang[3]; *[1]Tsinghua University, Beijing, China; [2]Peking University, Beijing, China; [3]The Hong Kong University of Science and Technology, Hong Kong, Hong Kong*

ThP 165 **Detection of cocaine derivatives in saliva in 45 seconds: combination of Probe ElectroSpray Ionization (PESI) and quadrupole time-of-flight (QTOF)**; Franck SAINT-MARCOUX[1]; Elisa JOUSSELIN[1]; Pauline GRIFFEUILLE[1]; Elies ZARROUK[1]; Souleiman EL BALKHI[1]; *[1]University Hospital of Limoges, Limoges, France*

ThP 166 **Paradigm shift in biomarker translation: an innovative and automated pipeline to generate and select clinical-grade signature peptides during DIA discovery**; Qin Fu[1]; Manasa Vegesna[1]; Niveda Sundararaman[1]; Eugen Damoc[2]; Tabiwang N Arrey[2]; Anna Pashkova[2]; Dalin Li[1]; Jonathan Braun[1]; Dermot P.B. McGovern[1]; Kermit K. Murray[1]; Xuan Yue[2]; Jennifer E. Van Eyk[1]; *[1]Cedars-Sinai Medical Center, Los Angeles, CA; [2]Thermo Fisher Scientific, Bremen, Germany*

ThP 167 **Parallel Reaction Monitoring for Quantitative Detection of Botulinum Neurotoxins in Complex Matrices**; Rose S Atukunda[1]; Karine Bagramyan[1]; Victoria Qiu[1]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA*

ThP 168 **Nausea and vomiting in pregnancy is caused by GDF15 produced by the fetus, not the mother**; Amy L George[1]; Emma Cook[2]; Steve D.S Charnock-Jones[2]; Frank Reimann[1]; Fiona M Gribble[1]; Gordon C.S Smith[2]; Stephen O'Rahilly[1]; Richard G Kay[3]; *[1]Wellcome Trust MRC Institute of Metabolic Science, Cambridge, United Kingdom; [2]Department of Obstetrics and Gynaecology, University of Cambridge, Cambridge, United Kingdom; [3]Wellcome Trust MRC Institute of Metabolic Science, Cambridge, United Kingdom*

ThP 169 **Selective and Sensitive Analysis of A6-peptide from Mouse Plasma Using LC MS/MS System**; Fatemeh Mousavi[1, 2]; Dan Su[1, 2]; *[1]HD Biosciences, San Diego, CA; [2]WuXi AppTec, SAN DIEGO, California*

ThP 170 **Medical applications of in vivo chemical biopsy probes based on sorbent coated acupuncture needles coupled with LC-MS and direct MS**; Runshan W Jiang[1]; Wei Zhou[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON*

ThP 171 **Simultaneous determination of three mAbs in human plasma by protein G magnetic beads extraction combined with LC-MS/MS**; Fengmei Hu[1]; Dan Liu[2]; Chao Huang[2]; Xianglong Zhao[2]; Lihai Guo[2]; *[1]Shanghai AB Sciex Analytical Instrument Trading Co.,Ltd., Shanghai, China; [2]SCIEX, Shanghai, China*

ThP 172 **24/7 fully automated therapeutic drug analysis for research projects by LC/MS/MS**; Aurore Jaffuel[1]; Frank Streit[2]; Kohei Yoshikawa[1]; *[1]Shimadzu Corporation, Nakagyo-ku, Japan; [2]Department of Clinical Chemistry, University Medical Center Goettingen, Goettingen, Germany*

ThP 173 **Improvement of system and methods for point-of-care testing of therapeutic drugs with miniature mass spectrometer**; Nan Zhang[1]; Mengyue Xu[1]; Weixu Fan[1]; Jian Zhao[1]; Yuyu Li[1]; Jiexun Bu[1]; Wenpeng Zhang[2]; Zheng Ouyang[2]; *[1]Purspec Technology (Beijing) Ltd., Beijing, China; [2]Tsinghua University, Beijing, China*

ThP 174 **Trace level determination of Polycyclic Aromatic Hydrocarbons in blood plasma using GC-MS/MS**; Santosh Kumar Bhardwaj[1]; Satyendra Pratap Singh Thakur[2]; Mohit Sharma[1]; Jitendra Kelkar[2]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., New Delhi, India; [2]Shimadzu Analytical (India) Pvt Ltd, New Delhi, India*

ThP 175 **Using the MSPen Technology for Intraoperative Identification of High-Grade Serous Carcinoma Metastatic Sites During Ovarian Cancer Surgeries**; Charles A. Wolfe[1]; Michael F. Keating[1, 2]; Monica Lin[1]; Ashley E. Montgomery[1]; Barrett C. Lawson[3]; Anil K. Sood[3]; Kelly Rangel[3]; Nicole D. Fleming[3]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Houston, TX; [2]University of Texas at Austin, Austin, TX; [3]MD Anderson Cancer Center, Houston, TX*

ThP 176 **LC-MS/MS assay for simultaneous quantification of antibiotics in sepsis therapy with efficient purification of clinical samples**; Alina Frieling[1, 2]; Nafissa Agardouh[3]; Malte Bayer[1, 2]; Thilo Bracht[1, 2]; Björn Koos[1]; Hartmuth Nowak[1]; Tim Rahmel[1]; Michael Adamzik[1]; Barbara Sitek[1, 2]; *[1]Clinic for Anesthesiology, Intensive Care and Pain Therapy, University Medical Centre, Knappschaftskrankenhaus Bochum, Bochum, Germany; [2]Medical Proteom-Centre, Ruhr-University Bochum, Bochum, Germany; [3]Ruhr-University Bochum, Faculty of Biology, Bochum, Germany*

ThP 177 **SLIMming Down the Workflow: A Novel Approach for Urine Toxicology Analysis**; Miriam Fico[1]; Zongyuan Chen[1]; Alan McKenzie-Coe[1]; Lauren Royer[1]; Joshua K. McBee[1]; Daniel DeBord[1]; Frederick G. Strathmann[1]; *[1]MOBILion Systems, Chadds Ford, PA*

ThP 178 **A sensitive LC-MS/MS method for relugolix quantification in human plasma and its application to a clinical study**; Sarah Lee[1]; Lan Li[2]; Yuan-Shek Chen[2]; Yu-Luan Chen[1]; *[1]Sumitomo Pharma America, Inc, Marlborough, MA; [2]QPS, LLC, Newark, DE*

ThP 179 **Quantitation of free amino acids in human plasma by Single Quadrupole LC-MS**; TUNA ONCU[1]; Oben Arslan[1]; Ugur Seker[1]; Huseyin Akpinar[1]; *[1]Shimadzu Middle East and Africa FZE Istanbul, Istanbul, Turkey*

ThP 180 **Pilot study of muscle aging in an older Indian cohort using Metabolomics**; Maroof Athar Hashmi[1]; Arvind Ramanathan[1]; *[1]Institute For Stem Cell Science and Regenerative Medicine, Bengaluru, India*

ThP 181 **An Automated Sample Preparation Approach for the Determination of Per- and Polyfluoroalkyl Substances (PFAS) from Human Biological Fluids using UHPLC-MS/MS**; Adam Senior[1]; Kyle Bevan[1]; Lee Williams[1]; Geoff Davies[1]; Alan Edgington[1]; Helen Lodder[1]; Russell Parry[1]; Lucy Lund[1]; Zainab Khan[1]; Claire Desbrow[1]; Dan Menasco[1]; *[1]Biotage GB Limited, Cardiff, United Kingdom*

ThP 182 **A 2D Microfluidic Paper-Based Analytical Device for Diagnosis of Canine Visceral Leishmaniasis in Developing Countries**; Hianka J. C. De Carvalho[1, 2]; Ayesha Seth[2]; Ruth M. Speidel[2]; Maria A. Miglino[1]; Abraham K. Badu-Tawiah[2]; *[1]Universidade de Sao Paulo, Sao Paulo, Brazil; [2]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio*

ThP 183 **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 184 **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[1]; Candace Fowler[2]; Benoît Denhez[3]; Pierre-Luc Mallet[3]; *[1]Université de Sherbrooke, Sherbrooke, QC; [2]Eastern Health, St. John's, NL; [3]CIUSSSE-CHUS, Sherbrooke*

ThP 185 **EXPANDING STEROID PROFILING BY UHPLC-MS/MS ANALYSIS OF ENDOGENOUS HORMONES AND PHASE II METABOLITES: INVESTIGATION OF CIRCADIAN VARIATIONS**; Federico Ponzetto[1]; Mirko Parasiliti-Caprino[1]; Laura Leoni[2]; Lorenzo Campioni[1]; Lorenzo Marinelli[1]; Fabio Settanni[3]; Antonello Nonnato[3]; Ezio Ghigo[1]; Roberta Giordano[4]; Giulio Mengozzi[2, 3]; *[1]Endocrinology, Diabetology and Metabolism, Department of Medical Sciences, University of Turin, Turin, Italy; [2]Clinical Biochemistry Laboratory, Department of Medical Sciences, University of Turin, Turin, Italy; [3]Clinical Biochemistry Laboratory, City of Health and Science University Hospital, Turin, Turin, Italy; [4]Department of Clinical and Biological Sciences, University of Turin, Turin, Italy*

ThP 186 **Empower the Quantitation of Amino Acids and Acylcarnitine for Inborn Error of Metabolism using Flow Injection – Orbitrap Mass Spectrometer**; Jingshu Guo[1]; Yvonne Song[1]; Kerry Hassell[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 187 **LC-MS/MS Screening Tests for Drug Abuse: Three Years of Experience at A Tertiary Hospital in Korea**; Ju Hyeong Lee[1]; Ayeong Bak[1]; Jongsun Joo[1]; Jikyo Lee[1]; Sang Hoon Song[1]; *[1]Seoul National University Hospital, Seoul, South Korea*

ThP 188 **Integrating Genomics, Proteomics, and Metabolomics Data within the NIH Multi-Omics for Health and Disease Consortium**; Cassandra G Kempf[1, 2]; Ethan Stancliffe[3]; Michaela Schwaiger-Haber[1]; Dhanalakshmi S Anbukumar[1]; Leah P Shriver[1, 2, 4]; Gary J. Patti[1, 2, 4]; *[1]Department of*

Chemistry, Washington University in St. Louis, Saint Louis, MO; [2]Center for Proteomics, Metabolomics and Isotope Tracing, Washington University in St. Louis, St. Louis, MO; [3]Panome Bio, St Louis, MO; [4]Department of Medicine, Washington University in St. Louis, Saint Louis, MO

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ThP 189 **Nitrile-Imine Crosslinking in Gas-Phase Peptide Ion Scaffolds**; Hongyi Zhu[1]; Kim Vu[1]; Marianna Nytka[2]; Karel Lemr[2, 3]; František Tureček[1]; *[1]University of Washington, seattle, WA; [2]Department of Analytical Chemistry, Faculty of Science, Palacký University, Tr. 17. listopadu 12, 779 00, Olomouc, Czech Republic; [3]Institute of Microbiology of the Czech Academy of Sciences, 142 20, Prague, Czech Republic*

ThP 190 **Quantitative Amine to Acid Chemical Crosslinking: Towards the Completion of the Conformationome of Alpha-Synuclein and its Proteoforms**; Ashlyn N Dollar[1]; Ian K Webb[1]; *[1]Indiana University Indianapolis, Indianapolis, IN*

ThP 191 **A covalent labeling-mass spectrometry based method for high-throughput screening of amyloid inhibitors**; Kanitin Khamnong[1]; Richard Vachet[1]; *[1]Department of Chemistry, University of Massachusetts Amherst, Amherst, MA*

ThP 192 **Characterization of Protein Structure by Top-Down Cleavable Crosslinking**; Erika Renbarger[1]; Ian K Webb[1]; *[1]Indiana University Indianapolis, Indianapolis, IN*

ThP 193 **Covalent Labeling Mass Spectrometry of a Membrane Protein on Live Cells Using a Label Enrichment Strategy**; Ina De La Fuente[1]; Elise Blackstock[1]; Richard Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

ThP 194 **LC separation optimization for XL-MS Analysis**; Yi He[1]; Erum Raja[2]; Leigh Foster[2]; Max Ruwolt[3]; Anthony Ciancone[4]; Fan Liu[3]; Francis O'Reilly[4]; Ryan Bomgarden[2]; Rosa Viner[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Rockford, Illinois; [3]Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; [4]NIH, Frederick, MD*

ThP 195 **Automated Hydroxyl Radical Protein Footprinting in a 96-Well Format**; Jiana Duan[1]; Zhi Cheng[1]; Emily Hart[1]; Casey Y. O'Connell[1]; Armando Santos-Landa[1]; Calyx Liu[1]; Robert Egan[1]; Joshua S Sharp[1, 2]; Scot Weinberger[1]; *[1]GenNext Technologies, Half Moon Bay, CA; [2]UNIVERSITY OF Mississippi, Oxford, MS*

ThP 196 **Fast and accurate disulfide bridge detection**; Richard Scheltema[1]; Søren Heissel[2]; Yi He[3]; Andris Jankevics[1]; Henrik Molina[2]; Rosa Viner[3]; *[1]Liverpool University, Liverpool, United Kingdom; [2]Proteomics Resource Center, The Rockefeller University, New York, New York; [3]ThermoFisher Scientific, San Jose, CA*

ThP 197 **Studying the Tau and Low-Density Lipoprotein Receptor-Related Protein 1 complex interface through Diethylpyrocarbonate - Based Covalent Labeling Mass Spectrometry**; Vanessa L. Stahl[1]; Trisha W. Brady[2]; Zachary J. Kirsch[2]; Jennifer N. Rauch[1, 3]; Richard W. Vachet[1, 2]; *[1]Molecular & Cellular Biology Program, University of Massachusetts Amherst, Amherst, MA; [2]Department of Chemistry, University of Massachusetts Amherst, Amherst, MA; [3]Department of Biochemistry & Molecular Biology, University of Massachusetts Amherst, Amherst, MA*

ThP 198 **Comparing an Epitope Identified from a Crystal Structure with In-solution Mass Spectrometry-based Techniques Including HRPF and XL-MS**; Zhi Cheng[1]; Emily Chea[1]; Rosa Viner[2]; Rodney G. King[3]; Guang Yang[3]; R. Glenn King[3]; Todd J. Green[3]; John T. Killian, Jr. [3]; Peter E. Prevelige[3]; Frances E. Lund[3]; Scot Weinberger[1]; *[1]GenNext Technologies, Half Moon Bay, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]University of Alabama Birmingham, Birmingham, Alabama*

ThP 199 **A Novel Crosslinker Improves Monolink and Crosslink Identification for Alphafold2 based Integrative Protein Structure Determination Pipeline**; Kish R. Adoni[1]; Karen Manalastas-Cantos Manalastas-Cantos[2]; Matthias Pfeifer[2]; Saad Shaaban[3]; Birgit Martens[2]; Bogdan R. Brutiu[3]; Kay Grunewald[2]; Nuno Maulide[3]; Maya Topf[2]; Konstantinos Thalassinos[1]; *[1]University College London, London, United Kingdom; [2]Centre for Structural Systems Biology, Hamburg, Germany; [3]University of Vienna / Department of Chemistry / Institute of Analytical Chemistry, Vienna, Austria*

ThP 200 **Cross-linking coupled to mass spectrometry (XLMS) for structural elucidation of antimicrobial peptide complexes: example of PGLa/Mag2**; Emilie Hirschler[1]; Elise Glattard[2]; Yannis-Nicolas François[1]; Burkhard Bechinger[2]; Emmanuelle Leize-Wagner[1]; Noelle Potier[1]; *[1]Laboratoire de spectrométrie de masse des interactions et des systèmes, UMR 7140, University of Strasbourg, Strasbourg, France; [2]Laboratoire de biophysique des membranes et RMN, UMR 7177, University of Strasbourg, Strasbourg, France*

ThP 201 **Identification of acidic amino acid side chains in proteins by selective chemical labeling and tandem mass spectrometry**; Akash Talukder[1]; Ashima Mehta[1]; Aisosa Omere[1]; Sepideh Khaki Firooz[1]; Joseph Anthony Buonomo[1]; Saiful M Chowdhury[1]; *[1]University of Texas at Arlington, Arlington, TX*

ThP 202 **Constructing a FPOP Spectral Library for Accurate Identification of Modified Amino Acids**; Haolin Luo[1]; Nuno Bandeira[2, 3, 4]; Lisa M. Jones[1]; *[1]Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA; [2]Center for Computational Mass Spectrometry, University of California San Diego, La Jolla, CA; [3]Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [4]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

ThP 203 **Discovering Crosslinks with Parallel Reaction Monitoring**; Lindsey D. Ulmer[1]; Lucas Narisawa[1]; Christopher N. Woods[2]; Natalie L. Stone[2]; Maria K. Janowska[2]; Rachel E. Klevit[2]; Matthew F. Bush[1]; *[1]Department of Chemistry, University of Washington, Seattle, WA; [2]Department of Biochemistry, University of Washington, Seattle, WA*

ThP 204 **Conventional cell fixation improves performance of in situ crosslinking mass spectrometry while preserving cellular ultrastructure.**; Andrew RM Michael[1]; Bruno C Amaral[1]; David C Schriemer[1]; *[1]University of Calgary, Calgary, AB*

ThP 205 **In-Cell Structural Determination of NFkB Inhibition by IkBa**; Luis Oliva[1]; Lisa M. Jones[1]; Elizabeth A. Komives[1]; *[1]University of California San Diego, La Jolla, CA*

ThP 206 **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[1, 2]; Alexandre GEFFROY[1, 2]; Fabrice BERTILE[1, 2]; Sarah Cianferani[1, 2]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, IPHC UMR 7178, Université de Strasbourg, CNRS, Strasbourg, France; [2]Infrastructure Nationale de Protéomique ProFI – FR2048, Strasbourg, France*

ThP 207 **Trapped-ion mobility spectrometry with PASEF for identification and quantification of protein-RNA crosslinks**; Sergey Moshkovskii[1]; Olexandr Dybkov[1]; Timo Sachsenberg[2, 3]; Ralf Pflanz[1]; Monika Raabe[1]; Oliver Kohlbacher[2, 3, 4]; Henning Urlaub[1, 5]; *[1]Bioanalytical Mass Spectrometry Group, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; [2]Applied Bioinformatics, Dept. of Computer Science, University of Tübingen, Tübingen, Germany; [3]Institute for Bioinformatics and Medical Informatics, University of Tubingen, Tubingen, Germany; [4]Institute for Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany; [5]Bioanalytics, Department of Clinical Chemistry, University Medical Center Göttingen, Göttingen, Germany*

ThP 208 **Inter-species click-linking: an improved strategy to estimate false discovery rates for protein-protein interactions detected by XL-MS**; Alex Crowder[1]; Bruno C Amaral[1]; Morgan Khan[1]; Pauline Douglas[1]; David C Schriemer[1]; *[1]University of Calgary, Calgary, AB*

ThP 209 **Navigating IgG-antiCH1 Binding Landscapes with Integrated Protein Footprinting Techniques to Assist Streamlined Purification Development**; Pengyi Zhao[1]; Yu Shi[1]; *[1]AstraZeneca, Gaithersburg, MD*

ThP 210 **Alzheimer's disease related amyloid-beta misfolding studied by gas-phase carbene footprinting mass spectrometry**; Paul Martino; *Houghton University, Houghton, NY*

ThP 211 **Probing the structural surfaceome of cancer cell models to identify tumor-specific protein conformations**; Audrey A Kishishita[1]; Abhilash Barpanda[1]; Arthur Zalevsky[1]; Deeptarup Biswas[2]; Ayushi Verma[2]; Sanjyot Vinayak Shenoy[2]; Michael R Hoopmann[3]; Clinton Yu[4]; Fenglong Jiao[4]; Lan Huang[4]; Robert L Moritz[3]; Andrej Sali[1]; Sanjeeva Srivastava[2]; Arun P Wiita[1]; *[1]UCSF, San Francisco, CA; [2]IIT Bombay, Mumbai, India; [3]Institute for Systems Biology, Seattle, Washington; [4]UCI, IRVINE, CA*

ThP 212 **Assessing a tyrosine-reactive functionality for covalent labeling and crosslinking applications: Introducing novel reagents for protein structural and interaction studies**; Saiful Chowdhury[1]; Adway Ouseph Zacharias[2]; Sharel Cornelius[2]; *[1]Univerisity of Texas at Arlington, Arlington, TX; [2]University of Texas at Arlington, Arlington, TX*

ThP 213 **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[1]; Ritchie Ly[2]; Clementina Strozek[2]; Paolo Cifani[3]; Michelle Sao[2]; Travis Hartman[2]; Justin R Cross[2]; *[1]Health Outlook, New York, NY; [2]Memorial Sloan Kettering Cancer Center, New York, NY; [3]Cold Spring Harbor Laboratory, Cold Spring Harbor, NY*

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ThP 214 **Validation of PROTAC drug targets with mass spectrometry-based quantitative proteomics method**; Zhiya Fan; *National Center for Protein Science, Beijing, Beijing, China*

ThP 215 **Novel mass spectrometry-based immuno-immobilization functional assay for the structure-activity relationship determination of modulators for a transmembrane sterol isomerase**; Reza Nemati Josheghani[1]; Ronghai Cheng[1]; Meiyi Zhang[2]; Daniel Tekverk[1]; Howard Jones[1]; Martin Himmelbauer[1]; *[1]Biogen, Cambridge, MA; [2]Texas A&M, College Station, TX*

ThP 216 **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 217 **A Validated HILIC-HRMS Method for Quantitative Analysisof Synthetic Oligonucleotides**; Md Rabiul Islam[1]; A M Abdullah[1]; Cynthia Sommers[1]; Jason Rodriguez[1]; Deyi Zhang[2]; Darby Kozak[2]; Kui Yang[1]; *[1]U.S. Food and Drug Administration, St. louis, MO; [2]U.S. Food and Drug Administration, Silver Spring, MD*

ThP 218 **High-Throughput Mass Spectrometry Based Screening Approach for Quantitative Protein-Ligand Affinity Measurements in Pooled Compound Libraries**; Craig B Gutierrez[1]; Neal Liddle[1]; Feizhi Ding[1]; Nomaan Rezayee[1]; Fred Manby[1]; Hui Zhang[1]; *[1]Iambic Therapeutics, San Diego, CA*

ThP 219 **Quantitative Analysis of Dithiothreitol (DTT) and Oxidized DTT in Three Acidified Cell Culture Media by LC/MS/MS**; Wen Lin[1]; Timothy White[1]; Erika Stark[1]; *[1]Charles River Laboratories, Worcester, MA*

ThP 220 **Systematic identification and validation of degrader drug targets by deep proteomic screening and high-sensitivity ubiquitinomics**; Uli Ohmayer[1]; Martin Steger[1]; Björn Schwalb[1]; Gisele Nishiguchi[2]; Kevin McGowan[2]; Jutta Fritz[1]; Vadim Demichev[3]; Zoran Rankovic[2]; Henrik Daub[1]; *[1]NEOsphere Biotechnologies GmbH, Planegg, Germany; [2]Department of Chemical Biology & Therapeutics, St. Jude Children's Research Hospital, Memphis, TN; [3]Charité, Universitätsmedizin Berlin, Berlin, Germany*

ThP 221 **Discovery of a novel, gut microbial small molecule that improves immunotherapy response in mice with humanized microbiomes**; Jasmine Chong[1]; Cuong Nguyen[1]; Greg Fedewa[1]; Leslie Sedgeman[1]; Antonio Carmona[1]; Miriam Velez[1]; Nathan Wan[1]; Yan Yang[1]; Sarkis Mazmanian[2]; Bryan Yoo[1]; *[1]Nuanced Health, Los Angeles, CA; [2]California Institute of Technology, Pasadena, CA*

ThP 222 **Characterization of antibody coverage for anti-HCP ELISA by nanoLC-MS/MS**; Jia Guo[1]; Yiran Liang[1]; Regina Kufer[2]; Stefanie Wohlrab[2]; Midori Greenwood-Goodwin[1]; Feng Yang[1]; *[1]Genentech, South San Francisco, CA; [2]Roche Diagnostics GmbH, Penzberg, Germany*

ThP 223 **LC-MS/MS quantification of total IgG of intravenous immunoglobulin (IVIg) in mouse plasma**; Dominic Bounkhoun[1]; Jose Trinidad[1]; Hsin Chen[1]; Weixuan Chen[1]; *[1]Johnson and Johnson, San Diego, CA*

ThP 224 **Detecting protein-protein interaction directly using crosslinking and high-mass MALDI mass spectrometry for SARS-CoV-2 drug discovery**; Congrui Tan[1]; Yuye Zhou[1, 2]; Renato Zenobi[1]; *[1]ETH Zurich, Zurich, Switzerland; [2]KTH Royal Institute of Techonology, Stockholm, Sweden*

ThP 225 **Label-free native MS-based screening of PROTACs and molecular glues**; Edvaldo V. S. Maciel[1]; Christian Meyners[1]; Felix Hausch[1]; Tanja Habeck[1]; Frederik Lermyte[1]; *[1]Technical University of Darmstadt, Clemens-Schöpf-Institute for Organic Chemistry and Biochemistry, Darmstadt, Germany*

ThP 226 **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[1]; Ashley Davie[1]; Elaine To[1]; Yurong Lai[1]; *[1]Gilead Sciences Inc., Foster City, CA*

ThP 227 **Using chiral derivatization, LC-HRMS, and SFC-MS/MS to mitigate the bioanalytical selectivity issue caused by the presence of isobaric interferences**; Kasie Fang[1]; Hermes Licea-Perez[1]; Timothy Sikorski[1]; *[1]GSK, Collegeville, PA*

ThP 228 **iBA (intelligent BioAnalysis): Pioneering the Future of Bioanalysis**; Romina Schnegotzki[1]; Svenja Mayer-Wrangowski[1]; Siegfried Wild[1]; Anne-Michaela Kuebler[1]; Wolfgang Joerg[2]; Juergen Weber[2]; Christian Spaeth[2]; Christoph Disch[2]; Andreas H. Luippold[1]; *[1]Drug Discovery Sciences, DDS, Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach, Germany; [2]Lab Equipment Solutions, LES, Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach, Germany*

ThP 229 **A High Throughput and Robust Assay for Quantifying a Bi-Specific Peptide Drug Conjugate (CRCPAC90387) in Human Plasma Using HPLC-MS/MS**; Limin Chu[1]; Robert Huang[2]; Hongfang (Andy) Xue[1]; Mo Xu[2]; Laixin Wang[1]; Guitao Wang[2]; Yuehui Ma[1]; Fan Pan[2]; Aining Li[2]; Aihua Liu[1]; *[1]Resolian (Formally Alliance Pharma), Malvern, PA; [2]Coherent Biopharma, Hefei, China*

ThP 230 **Development of a high-throughput tissue sample processing approach for CETSA MS**; Mariel Grace R Mendoza[1]; Matthew Mazur[1]; Christopher Novotny[2]; Anu Sebin[2]; Weixun Wang[1]; *[1]Merck & Co., Inc., West Point, PA; [2]Merck, South San Francisco, CA*

ThP 231 **Parallel Global Metabolite Profiling and Characterization of Potential Drug Metabolites in Three-dimensional Hepatospheroids**; Darshak Gadara[1, 2, 3]; Songjie Chen[4]; Leah P. Shriver[1, 2, 3]; Thuy Tran[4]; Oscar Ekpenyong[4]; Dan Rock[4]; Gary J. Patti[1, 2, 3]; *[1]Department of Chemistry, Washington University in St. Louis, Saint Louis, MO; [2]Center for Proteomics, Metabolomics and Isotope Tracing, Washington University in St. Louis, Saint Louis, MO; [3]Department of Medicine, Washington University in St. Louis,* *Saint Louis, MO; [4]Department of Pharmacokinetics, Dynamics, Metabolism and Bioanalytics, Merck & Co., Inc., South San Francisco, CA*

ThP 232 **A Proteomics-Based Platform for High-Throughput Screening of Kinase Inhibitors**; Ravi Tharakan[1]; Yanyan Qu[1]; Yuhong Fang[1]; Patrick J. Morris[1]; Michele Ceribelli[1]; Craig J Thomas[1]; Christopher A LeClair[1]; Dingyin Tao[1]; *[1]National Center for Advancing Translational Sciences, NIH, Rockville, MD*

ThP 233 **Role of density functional theory in explaining MS/MS fragmentation mechanism of biologically active substituted urea derivative quizartinib**; Sudam S Mane[1]; David V Dearden[1]; *[1]Brigham Young University, Provo, UT*

ThP 234 **Auranofin targets UBA1 and enhances activity by facilitating ubiquitin transthioesterification to E2 ubiquitin conjugating enzymes**; Dingyin Tao[1]; Yanyan Qu[1]; Christopher A LeClair[1]; Shengyun Fang[2]; *[1]National Center for Advancing Translational Sciences, NIH, Rockville, MD; [2]University of Maryland, Baltimore, Baltimore, MD*

ThP 235 **A simple, direct and sensitive LC-MS/MS method for the determination of cationic lipid in human liver microsomes**; Jiao Zhang[1]; Dan Li[1]; Yangzhen Zheng[1]; Juanjuan Zhu[1]; Jinlian Lu[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

ThP 236 **Deploying an Ultra-Sensitive, High-Throughput, Integrated Microflow LC-MS/MS System to Support in vitro PK/PD Assessment**; Brendon Kapinos[1]; Jamie Tourville[1]; Qianying Yuan[1]; Ashley Bertrand[1]; Mitchell Laughlin[1]; Tom Schroeter[1]; Steve Ainley[2]; Wayne Lootsma[2]; *[1]Pfizer, Groton, CT; [2]Sound Analytics, Deep River, CT*

ThP 237 **Isotyping and quantitation of anti-AAV antibody in human serum by immunoprecipitation coupled to liquid chromatography and mass spectrometry**; Xiaoxiao Huang[1]; Yuetian Yan[1]; Sven Moller-Tank[1]; Shunhai Wang[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals, Tarrytown, NY*

ThP 238 **Development of a Validated LC-MS/MS Method for the Quantification of Psilocin in Mouse Plasma: Addressing a Major Interference**; Amir Khajavinia[1]; Deborah Michel[1]; Udoka C Ezeaka[1]; Randy W Purves[1, 2]; Robert B Laprarie[1]; Anas El-Aneed[1]; *[1]University of Saskatchewan, Saskatoon, SK; [2]Canadian Food Inspection Agency, Saskatoon, SK*

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ThP 240 **Utilization of Immunoprecipitation to Assess H3.3K36M Oncohistone Proteoforms and Post-Translational Modifications for Quantitative Top-Down Mass Spectrometry**; Alyssa Paparella[1]; Karl F. Poncha[1]; Cheryl L. Walker[1]; Nicolas L. Young[1]; *[1]Baylor College of Medicine, Houston, TX*

ThP 241 **Systematic Characterization of Recombinant and Endogenous Chlamydomonas reinhardtii SET-Domain Methyltransferases by Biochemical and Mass Spectrometric Approaches**; Michael Hayes[1]; James J Pesavento[1]; *[1]Saint Mary's College, Moraga, CA*

ThP 242 **Identification of histone lysine acetoacetylation as a dynamic post-translational modification regulated by HBO1**; Yan Gao[1]; Xinlei Sheng[2]; Doudou Tan[3]; Sunjoo Kim[1]; He Huang[3]; Yingming Zhao[2]; Sangkyu Lee[4]; *[1]College of Pharmacy, Kyungpook National University, Daegu, South Korea; [2]The University of Chicago, Chicago, IL; [3]Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China; [4]School of Pharmacy, Sungkyunkwan University, Suwon, South Korea*

ThP 243 **An optimized workflow for monitoring the canonical histone ubiquitination marks H2AK119ub and H2BK120ub by LC-MS/MS**; Peder J. Lund[1]; Mariana Lopes[1]; Benjamin A. Garcia[2]; *[1]Department of Nutrition, Case Western Reserve University, School of Medicine, Cleveland, OH; [2]Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine, St. Louis, MO*

ThP 244 **Top down proteomics reveals a proteoform-truncation mechanism that supersedes the DNA damage and apoptotic response**; Faith M. Joseph[1]; Matthew V. Holt[1]; Nicolas L. Young[2]; *[1]Baylor College of Medicine, Houston, Texas; [2]Baylor College of Medicine, Houston, TX*

ThP 245 **Scoring Post-translational Modification Crosstalk from Histone Proteoform Data**; Karl F Poncha[1]; Alyssa T. Paparella[2]; Nicolas L. Young[1, 2, 3]; *[1]Verna and Marrs McLean Department of Biochemistry and Molecular Pharmacology, Baylor College of Medicine, Houston, TX; [2]Center for Precision Environmental Health, Baylor College of Medicine, Houston, TX; [3]Department of Molecular and Cellular Biology, Baylor College of Medicine, Houston, TX*

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ThP 246 **Quantification and Identification of Arsenic Species in Freshwater Fish Using HPLC-ICPMS/ESIMS**; Chester Lau[1]; Xiufen Lu[2]; Tetiana Davydiuk[1]; Jennifer A. Graydon[3]; Megan Reichert[3]; Ruth Mitchell[3]; X. Chris Le[1, 2]; *[1]Department of Chemistry, University of Alberta, Edmonton, AB; [2]Department of Laboratory Medicine and Pathology, University of Alberta, Edmonton, AB; [3]Alberta Health, Health Protection Branch, Edmonton, AB*

ThP 247 **Direct injection screening method for Per-and-polyfluoroalkyl substances in drinking water using a prototype benchtop multi-reflecting Time-of-flight**; Hania Khoury-Hollins[1]; Stuart Adams[1]; Jayne Kirk[1]; Richard Lock[1]; Lance Nicolaysen[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters, Milford, MA*

ThP 248 **Orbitrap isotopic ratio mass spectrometry of methylated stearic acid and its application to vegetable butter source discrimination**; Gabriel Franco Dos Santos[1]; Alexis Gilbert[2]; Giovanni B. Bevilaqua[1]; Hugo G. Machado[1]; Maxime Julien[3]; Gesiane S. Lima[1]; Nerilson M. Lima[1]; Júlio C. O. Ribeiro[1]; Alexandre A. Ferreira[4]; Ygor S. Rocha[4]; Boniek G. Vaz[1]; *[1]Federal University of Goias, Goiânia, Brazil; [2]Tokyo Institute of Technology, Tokyo, Japan; [3]Université de Nantes, CNRS, Nantes, France; [4]PETROBRAS, Rio de Janeiro, Brazil*

ThP 249 **Measuring per- and polyfluoroalkyl substances in baby formula powder: A quantitative LC-MS/MS approach**; Matthew Noestheden[1, 2]; Karl Oetjen[3]; Simon Roberts[3]; *[1]SCIEX, Concord, ON; [2]University of British Columbia, Vancouver, BC; [3]Sciex, Framingham, MA*

ThP 250 **Confirming veterinary drug residues in problematic samples using a rapid FAIMS-based strategy with existing diagnostic LC-MS methods**; Randall W Purves[1]; Michael W. Belford[2]; Bryn O. Shurmer[1]; Jana Kinar[1]; *[1]Canadian Food Inspection Agency, Saskatoon, SK; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 251 **Development of a high-resolution MRM quantitative method for pesticides in apple, honey, olive oil, orange and tomato food matrices**; Alan Barnes[1]; Raquel Leonardo[2]; Emily G Armitage[1]; Jonathan McGeehan[3]; Steve Williams[2]; Neil J Loftus[1]; *[1]Shimadzu Corporation, Manchester, United Kingdom; [2]SGS Cambridge Limited, Cambridge, United Kingdom; [3]Shimadzu UK Limited, Milton Keynes, United Kingdom*

ThP 252 **Quantitation of Zearalenone and Deoxynivalenol in Zea Mays using LC-MS**; Valeria Zerda-Pinto[1]; Charlette Hasty[2]; Mary-Margaret B Benware[1]; Tyson Lobb[1]; Ifeoluwa P Osikoya[1]; Fatima Romo[1]; Olufunke M Ayegbidun[1]; Logan M Stenger[3]; John A Juvik[3]; Laura A Chatham[3]; Tiffany M Jamann[3]; Anthony J Studer[3]; Martin O Bohn[3]; Carolyn Butts-Willmsmeyer[1]; Kevin Tucker[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL; [2]Southern Illinois University Carbondale, Carbondale, IL; [3]University of Illinois Urbana-Champaign, Champaign, IL*

ThP 253 **Determination of Ergot Alkaloids in Cereal-based Food using LC-MS/MS**; Weili Xiong[1]; Christian Talavera[1]; *[1]U.S. Food and Drug Administration, College Park, MD*

ThP 254 **An Integrated GC-MS/MS and LC-MS/MS Workflow for Quantitative Analysis of Pesticides with Cross-confirmation using a Single Chromatography Data System Software**; Ed George[1]; Julie Moriceau[2]; Delphine Thomas[3]; Jean-François Garnier[2]; Richard Fussell[4]; Toby Astill[1]; *[1]ThermoFisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermo Fisher Scientific GmbH, Bremen, Germany; [4]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*

ThP 255 **LC-MS/MS-based dilute-and-shoot approach for the quantitation of more than 800 pesticides and mycotoxins: challenges and solutions**; Jianru Stahl-Zeng[1]; Hassan El Khallabi[2]; Jack Steed[3]; Said El Ouadi[4]; Ian Moore[5]; *[1]SCIEX, Darmstadt, Germany; [2]Normec Groen Agro Control, Delfgauw, Netherlands; [3]SCIEX UK, Macclesfield, United Kingdom; [4]SCIEX, Darmstadt, Germany; [5]SCIEX, Concord, ON*

ThP 256 **Utilizing hydrogen carrier gas for sensitive analysisof pesticides in food using gas chromatography mass spectrometry**; Adam Ladak[1]; Paul Silcock[2]; Xin Zheng[3]; Jason Cole[3]; Amit Gujar[3]; Daniel Kutscher[4]; Nicholas Warner[4]; *[1]Thermo Scientific, Macclesfield, United Kingdom; [2]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [3]Thermo Fisher Scientific, Bannockburn, IL; [4]Thermo Fisher Scientific, Bremen, Germany*

ThP 257 **A Dietary Glycan Encyclopedia of Food: Unveiling Molecular Structures via LC-MS for Precision Nutrition Initiatives**; Shawn Ehlers-Cheang[1]; Christopher Suarez[1]; Jules A Larke[2, 3]; Jiani Jiang[1]; Cheng-Yu Charlie Weng[1]; Aaron D Stacy[1]; Danielle G Lemay[2, 3]; Carlito B. Lebrilla[1]; *[1]Department of Chemistry, University of California, Davis, Davis, CA; [2]Department of Food Science and Technology, University of California, Davis, Davis, CA; [3]Western Human Nutrition Research Center, USDA Agricultural Research Service, Davis, CA*

ThP 258 **Determination of 31 Per- and Poly-fluoroalkyl Substances in Food Packaging with APGC-MS/MS and UPLC-MS/MS**; Chia-Yang Chen[1, 2]; I-Chieh Hu[2]; *[1]Institute of Food Safety and Health, National Taiwan University, Taipei City, Taiwan; [2]Institute of Environmental and Occupational Health Sciences, National Taiwan University, Taipei City, Taiwan*

ThP 259 **Method Validation for Determining 513 Pesticide Residues in Cucumber Using LCMS-8060NX and 308 Residues by GCMS-TQ8040NX**; Anant Lohar[1]; Rakan Saad Abdullah Alajmi[2]; Hatim Zaid Ali Alhazmi[2]; Sarah Awwadh Sultan Alotaibi[2]; Jayachandran Namasivayam[3]; Shailesh Damale[1]; Jessin Mathai[1]; *[1]Shimadzu Middle East and Africa FZE, Dubai, United Arab Emirates; [2]Saudi Food and Drug Authority, Riyadh, Saudi Arabia; [3]AnalyticaOne Group, Doha, Qatar*

ThP 260 **Comparison of sample preparation for determination of mycotoxins in cannabis and cannabis derived products using LC-FLD and LC-MS/MS**; Giorgia Greco[1]; Juliane Kramer[1]; Susanne Huhmann[1]; *[1]KNAUER, Berlin, Germany*

ThP 261 **Ultra-fast multiresidues accurate mass screening strategy**; Olivier Chevallier[1]; Cate Simmermaker[1]; Kai Chen[1]; Chris Klein[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 262 **New model to optimize triple quadrupole mass spectrometer performance for fast SRM methods**; Michael Ugarov[1]; Harald Oser[1]; Hans Schweingruber[1]; Neloni Wijeratne[1]; Agnès Le Corre[2]; Claudia Martins[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Courtaboeuf, France*

ThP 263 **Sulfite Quantification in Foods and Beverages Using Single Quadrupole LC-MS**; Saho Yoshioka[1]; Nozomi Maeshima[1]; Dominika Gruszecka[2]; Landon Wiest[2]; Ryo Yamaguchi[1]; Manami Kobayashi[1]; *[1]SHIMADZU Corporation, Kawasaki, Japan; [2]Shimadzu Scientific Instruments, Columbia, MD*

ThP 264 **Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Fish Fillet with LC-MS/MS**; Kota Ishioka[1]; Nozomi Maeshima[1]; Toshiya Matsubara[2]; Manami Kobayashi[1]; *[1]SHIMADZU Corporation, Kawasaki, Japan; [2]Shimadzu Scientific Instruments, Columbia, MD*

ThP 265 **Simultaneous Analysis of Pesticides in Food With GC-MS/MS Using Hydrogen Carrier Gas**; Nozomi Maeshima[1]; Kyoko Yamada[1]; Yoshihiro Saito[1]; Dominika Gruszecka[2]; Alan Owens[2]; Manami Kobayashi[1]; *[1]SHIMADZU Corporation, Kawasaki, Japan; [2]Shimadzu Scientific Instruments, Columbia, MD*

ThP 266 **Determination of mycotoxins in dry feed for small animals**; Laudicéia Alves De Oliveira[1]; Marcelo Viana De Moraes[2]; Edivaldo Domingues Velini[2, 3]; Ichiro Hirano[1]; Marcos Albieri Pudenzi[1]; *[1]Shimadzu do Brasil, Barueri, Brazil; [2]Bioativa, Botucatu, Brazil; [3]Universidade Estadual Paulista - UNESP, Botucatu, Brazil*

ThP 267 **Investigating Per- and Poly-Fluoroalkyl Substances (PFAS) Interferences in Food Matrices with High-Resolution Mass Spectrometry**; Brian Ng[1]; Christine M Fisher[1]; Susan Genualdi[1]; Wendy Young[1]; Elsie Peprah[1]; Lowri De Jager[1]; *[1]U.S. Food and Drug Administration, College Park, MD*

ThP 268 **Reliable determination of anionic polar pesticides in fruits and vegetables by using LC-MS/MS**; Samruddha Chavan[1]; Nitin Shukla[1]; Nitish Ramchandra Suryawanshi[1]; Nilesh Patil[1]; Ramesh Manigiri[1]; Shraddha Kadam[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

ThP 269 **Application of a Novel Automated Sample Preparation Platform for the Determination of Acrylamide in Instant Coffee and Analysis using UPLC-MS/MS**; Russell Parry[1]; Helen Lodder[1]; Alan Edgington[1]; Lee Williams[1]; Charlotte Hayes[1]; Geoff Davies[1]; Adam Senior[1]; Lucy Lund[1]; Zainab Khan[1]; Claire Desbrow[1]; Dan Menasco[1]; *[1]Biotage GB Limited, Cardiff, United Kingdom*

ThP 270 **Simultaneous Determination of Alternaria Toxins, Ergot Alkaloid Epimers, and Other Major Mycotoxins in Various Food Matrices by LC-MS/MS**; Diego A Lopez[1]; Shun-Hsin Liang[1]; Justin Steimling[1]; *[1]Restek Corporation, Bellefonte, PA*

ThP 271 **Mass spectrometric characterization of natural protein sweeteners for evaluation as substitutes for artificial sweeteners**; SEPIDEH KHAKI FIROOZ[1]; Saiful M Chowdhury[2]; *[1]University of Texas at Arlington (UTA), Arlington, TX; [2]University of Texas at Arlington, Arlington, TX*

ThP 272 **How to deal with sweet matrix? – a method for LC-MS/MS analysis of antibiotics in honey, regardless of its kind**; Julia Mironenka[1]; Rafal Szewczyk[1, 2]; Katarzyna Krupczyńska-Stopa[1, 2]; Maciej Stopa[1, 2]; *[1]LabExperts sp. z o.o. NIP:5833181181, Gdansk, Poland; [2]Bioanalytic sp z o.o., Gdańsk, Poland*

ThP 273 **Development of a QuEChERS-based UPLC-MS/MS for the Simultaneous Determination of Neonicotinoids, Parabens, and Bisphenols in Vegetables and Biscuits**; Hsin-Chang Chen[1]; Zou-Xiao Huang[2]; Jung-Wei Chang[3]; Po-Chin Huang[4, 5, 6]; *[1]Department of Chemistry, Tunghai University, Taichung City, Taiwan; [2]Institute of Food Safety and Health, National Taiwan University, Taipei City, Taiwan; [3]Institute of Environmental and Occupational Health Sciences, School of Medicine, National Yang Ming Chiao Tung University, Taipei, Taiwan; [4]National Institute of Environmental Health Sciences, National Health Research Institutes, Miaoli, Taiwan; [5]Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; [6]Department of Medical Research, China Medical University Hospital, China Medical University, Taichung City, Taiwan*

ThP 274 **Advanced Solid-Phase Extraction Methods for Rapid Pesticide Residue Analysis Compatible with Both GC-MS and LC-MS/MS, Utilizing QuEChERS Extraction**; Takumi Kunieda[1]; Manabu Takayanagi[1]; Shigenori Ota[1]; *[1]GL Sciences Inc., Saitama, Japan*

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ThP 275 **Rapid detection and classification of near-neighbor fentanyl variants by 2D MS/MS and machine learning**; Dalton Snyder[1]; Megan Guetzloff[1]; Jane Likens[1]; Anthony Eshleman[1]; Andrew Houvenagle[1]; Kevin Rosenbaum[1]; Austin Stieglitz[1]; Brandon Reese[1]; Mitch Wells[1]; *[1]Teledyne FLIR, West Lafayette, IN*

ThP 276 **Characterization of oligomeric 2-butanone peroxide species and the associated gas-phase and solution-phase rearrangement products by electrospray ionization**; Ryan M Bain[1]; John Stutzman[2]; Julie Pannuto[1]; Meghan Kane[1]; *[1]Bureau of Alcohol, Tobacco, Firearms and Explosives, Beltsville, MD; [2]Dow Inc, Midland, MI*

ThP 277 **Identification of Isobaric Methyl-Substituted Fentanyl Analogs using a Transportable Linear Ion Trap Mass Spectrometer**; Alleigh N. Couch[1]; J. Tyler Davidson[1]; *[1]Department of Forensic Science, Sam Houston State University, Huntsville, TX*

ThP 278 **Towards a Combined Spectroscopic/Spectrometric Approach for Processing Modern Forensic Drug Evidence**; Emily J. Wiggins[1]; Ebenezer H. Bondzie[1]; Jamie R. Wieland[1]; Jun-Hyun Kim[1]; Christopher Mulligan[1]; *[1]Illinois State University, Normal, IL*

ThP 279 **Enhanced Genetically Variant Peptide Profiling from Human Hair Using Keratinase and Trypsin**; Zheng Zhang[1]; William E. Wallace[1]; Guanghui Wang[1]; Meghan C. Burke[1]; Yi Liu[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

ThP 280 **Analysis of Explosives using Laser Diode Thermal Desorption (LDTD) coupled to a Orbitrap mass spectrometer**; Amanda Wriston[1]; Gina M. Guerrera[1]; Eshwar Jagerdeo[1]; *[1]FBI, Quantico, VA*

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ThP 282 **Illicit Drug Desorption and Chemical Profiling of Fingerprints using SICRIT Ion Source: A Rapid Analysis Approach**; Ciara Conway[1, 2]; Markus Weber[1, 2]; Allison Ferranti[2]; Jan-Christoph Wolf[2]; Christoph Haisch[1]; *[1]Technical University of Munich, Freising, Germany; [2]Plasmion GmbH, Augsburg, Germany*

ThP 283 **Simultaneous screening of nearly 300 synthetic cannabinoids and metabolites in blood and urine samples using an LC-QTOF system**; Jiahong Xiang[1]; Yan Shi[2]; Yukun Chen[3]; Zong Yang[3]; Bingjie Liu[3]; Lihai Guo[3]; *[1]College of Forensic Medicine, Hebei Medical University, Shijiazhuang, China; [2]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; [3]SCIEX Asia Pacific Application Support Center, Shanghai, China*

ThP 284 **Automated solid-phase extraction with gas chromatography-mass spectrometry for high-throughput analysis and application of narcotic drugs in human urine**; Chohee Jeong[1]; Hamin Choi[1]; Sang Beom Han[1]; *[1]Dept of Pharmaceutical Analysis, College of Pharmacy, Chung-Ang University, seoul, South Korea*

ThP 285 **Cannabinoids Isomeric Profiling in Seized Materials by LC-ESI(±)LTQ MS**; Wanderson Romao[1, 2]; João Victor M. De Almeida[3]; Nathália S. Conceição[2, 3]; Marcos Valério V. Lyrio[3]; Nayara A. dos Santos[2, 3]; Rafael S. Ortiz[2, 4]; *[1]Federal Institute of Espírito Santo, Brazil, Vitoria, Brazil; [2]National Institute of Forensic Science and Technology, INCT, Porto Alegre, Brazil; [3]Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espirito Santo, Vitória, Brazil; [4]Technical-Scientific Sector, Regional Superintendence of the Federal Police Department in Rio Grande do Sul, Brazil, Porto Alegre, Brazil*

ThP 286 **Simultaneous detection of cocaine and its metabolites in urine samples by direct analysis using Cellulose Fiber Spray Ionization Mass Spectrometry**; Nayara Araujo Dos Santos[1, 2]; Nathália dos Santos Conceição[1, 2]; Sara Joaquina I. Dionisio[1]; Emmily Travassos Alves[1]; Bruna Carneiro Pires[2]; Wanderson Romão[1, 2, 3]; *[1]Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espirito Santo, Vitória, Brazil; [2]National Institute of Forensic Science and Technology, INCT, Porto Alegre, Brazil; [3]Federal Institute of Espírito Santo, Brazil, Vila Velha, Brazil*

ThP 287 **Application of a novel screening workflow for the detection of illicit and medicinal drugs in human hair**; Emily G Armitage[1]; Thomas Brema[2]; Christopher Bowen[3]; Alan Barnes[1]; Rohan Steel[4]; Neil J Loftus[1]; *[1]Shimadzu Corporation, Manchester, United Kingdom; [2]Shimadzu Deutschland GmbH, Duisburg, Germany; [3]Shimadzu Scientific Instruments, Melbourne, Australia; [4]Biological Research Unit, Racing Analytical Services Limited, Flemington, Australia*

ThP 288 **Forensic Applications of a Validation and Implementation Package for Rapid GC-MS Analysis of Seized Drugs and Ignitable Liquids**; Briana A. Capistran[1]; Elizabeth L. Robinson[1]; Edward Sisco[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

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ThP 291 **A New Workflow for Fast Elucidation of Drug Metabolites for Screening – A Story of Microsomes and Microchips**; Annette Zschiesche[1]; Birgit Schneider[2]; Ilona Nordhorn[2]; Carsten Baessmann[2]; Laura M. Huppertz[1]; Jürgen Kempf[1]; *[1]Institute of Forensic Medicine, Medical Center - University of Freiburg, Freiburg, Germany; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

ThP 292 **Analyzing the chemical footprints of toxic and hazardous compounds in dust particles in real-time using Single-Particle Mass Spectrometry**; Heinrich Ruser[1]; Johannes Passig[2, 3]; Sven Ehlert[4]; Haseeb Hakkim[2]; Marco Schmidt[2]; Aleksandrs Kalamasnikovs[2]; Michael Pütz[5]; Petra Hehet[5]; Martin Seipenbusch[6]; Karsten Wegner[6]; Andreas Walte[4]; Ralf Zimmermann[2, 3]; *[1]University of the Bundeswehr Munich, Neubiberg, Germany; [2]University of Rostock, Rostock, Germany; [3]Joint Mass Spectrometry Centre, Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Munich, Munich, Germany; [4]Photonion GmbH, Schwerin, Germany; [5]Federal Criminal Police Office, Forensic Science Institute, Wiesbaden, Germany; [6]ParteQ GmbH, Malsch, Germany*

ThP 293 **Sensitive UHPLC-MS/MS and enantioselective SFC-MS method for determination of pharmakokinetic profiles of methoxphenidine and its metabolite in biological matrices**; Natalie Paškanová[1]; Magdalena Vagnerova[2]; Bronislav Jurásek[1]; Martin Kuchar[1]; Michal Kohout[3]; *[1]Department of Chemistry of Natural Compound and Forensic Laboratory of Biologically Active Substances, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic; [2]Department of Analytical Chemistry, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic; [3]Department of Organic Chemistry, UCT Prague, Technická 5, Prague 6 - Dejvice, Czech Republic*

ThP 294 **T-ReXing Synthetic Cannabinoid Receptor Agonists – Unveiling Metabolites Suitable for Urine Screening via UHPLC-timsTOF-MS and MetaboScape**; Annette Zschiesche[1]; Birgit Schneider[2]; Ilona Nordhorn[2]; Carsten Baessmann[2]; Jürgen Kempf[1]; Laura M. Huppertz[1]; *[1]Institute of Forensic Medicine, Medical Center - University of Freiburg, Freiburg, Germany; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

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ThP 296 **Rapid screening and quantitation of forensically-relevant samples using LC-timsTOF**; William J Feeney[1]; Edward Sisco[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

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ThP 299 **Detection of xylazine-laced fentanyl using a novel acoustic ejection HRMS**; Aaron Stella[1]; Jacob Watson McCabe[2]; Anuja Bhalkikar[2]; Babu Purkayastha[2]; *[1]SCIEX, Framingham, MA; [2]Sciex, Framingham, MA*

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ThP 354 **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[1]; Chee-Leong Kee[1]; Nuan-Ping Cheah[1]; Huishi Koh[1]; *[1]Health Sciences Authority, Singapore, Singapore*

ThP 355 **Exploiting GC(×GC)-HRMS capabilities for targeted and non-targeted analysis of (semi)volatile poly- & perfluorinated hydrocarbons in ambient air**; Maria Chiara Corvisieri[1]; Marco De Poli[2]; Claudia Stevanin[1]; Tatiana Chenet[1]; Alberto Cavazzini[2]; Luisa Pasti[1]; Flavio Antonio Franchina[2]; *[1]Department of Environmental and Prevention Sciences, University of Ferrara, Ferrara, Italy; [2]Department of Chemical, Pharmaceutical, and Agricultural Sciences, University of Ferrara, Ferrara, Italy*

ThP 356 **Meeting the challenges of Dioxin analysis and more with GC-Orbitrap high mass resolution capabilities**; Dominic Roberts[1]; Nicholas Warner[2]; Paolo Benedetti[3]; Xin Zheng[4]; Jason Cole[4]; Daniel Kutscher[5]; *[1]Thermo Fisher Scientific, Runcorn, United Kingdom; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermo Fisher Scientific, Milan, Italy; [4]Thermo Fisher Scientific, Austin, Texas; [5]Thermo Fisher Scientific, Bremen, Germany*

ThP 357 **Improved identification of extractable and leachable substances with Orbitrap Exploris GC 240**; Dominic Roberts[1]; Nicholas Warner[2]; Xin Zheng[3]; Jason Cole[3]; Dujuan Lu[4]; Chongming Liu[4]; Nan Zhang[4]; Sven Hackbusch[5]; Daniel Kutscher[6]; *[1]Thermo Fisher Scientific, Runcorn, United Kingdom; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermo Fisher Scientific, Austin, Texas; [4]SGS Health Science, Fairfield, New Jersey; [5]Thermo Fisher Scientific, San Jose, CA; [6]Thermo Fisher Scientific, Bremen, Germany*

ThP 358 **Comparison of Different Sample Preparation Techniques for Analyzing Volatile and semi-Volatile Organic Compounds in Recycled Plastics Using GC/MS**; Renzo Picenoni[1]; Tiantian Li[1]; Günter Böhm[1]; Stefan Cretnik[1]; *[1]CTC Analytics AG, Zwingen, Switzerland*

ThP 359 **Determination of six aromatic amines in the mainstream smoke of tobacco products**; Huihua Ji[1]; Zhenyu Jin[1]; *[1]University of Kentucky, Lexington, KY*

ThP 360 **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[1]; John Carpin[2]; *[1]U.S. Army CCDEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; [2]EXCET Incorporated, Edgewood, MD*

ThP 361 **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 362 **Faster Qualitative Analysis of Essential Oils Using GC/MS with Hydrogen CarrierGas and a Hydrogen Optimized EI Source**; Bruce Quimby[1]; Anastasia Andrianova[1]; Lakshmi Krishnan[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Santa Clara, CA*

ThP 363 **Fast Analysis of 140 Pesticides, PAHs, and PCBs by GC/MS/MS**; Erinn M ONeill[1]; Alexis Willey[1]; Marta Venier[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Indiana University, Bloomington, IN*

ThP 364 **Improving Emissivity Through Improved Yttria Coatings for GCMS Filaments**; Ron Shomo[1]; Kenneth Wright[1]; *[1]IMI ADAPTAS, Palmer, MA*

ThP 365 **Brewing Excellence: Quantitating Over 200 Pesticides in Black Tea with Steady Performance and Maximized Uptime**; Anastasia Andrianova[1]; Eric Fausett[1]; Bruce Quimby[1]; Limian Zhao[1]; Joel Ferrer[2]; Aaron Boice[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Santa Clara, CA*

ThP 366 **Enhanced Longevity and Revolutionized Robustness for Sensitive Detection of 190 Pesticides over 800 Injections with Novel HES 2.0 Source**; Brooke C Reaser[1]; Luis Cuadra-Rodriguez[1]; Elias Feresenbet[1]; Ge Yu[1]; Alexander Mordehai[1]; Nathan Eno[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 367 **Novel High Sensitivity Detector for GC/MS**; Hiroki Kannen[1]; Shun Kogiso[2]; Yoshiro Hiramatsu[3]; Alan Owens[3]; Masaru Nishiguchi[2]; *[1]Shimadzu, Kyoto, Japan; [2]Shimadzu Corporation, Kyoto, Japan; [3]Shimadzu Scientific Instruments, Columbia, MD*

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ThP 369 **Systematic investigation of the trafficking of glycoproteins on the cell surface**; Xing Xu[1]; Kejun Yin[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

ThP 370 **Mass Spectrometric Investigation of the Fragile X Glycoproteome in Developing Mice**; Elliot Patrenets[1]; Hannah N Miles[2]; Thao Duong[3]; Ashley Phetsanthad[3]; Pamela R Westmark[4, 5]; Cara J Westmark[4, 5]; Lingjun Li[2, 3, 5];

[1]University of Wisconsin-Madison, Department of Integrative Biology, Madison, Wisconsin; [2]University of Wisconsin-Madison, School of Pharmacy, Madison, Wisconsin; [3]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [4]University of Wisconsin Madison, Department of Neurology, Madison, Wisconsin; [5]University of Wisconsin Madison, Molecular Environmental Toxicology Center, Madison, Wisconsin

ThP 371 **Ultra-sensitive platelet proteome identifies a new form of domain-specific O-fucosylation generated by FUT10 and FUT11**; Huilin Hao[1]; Callum B Houlahan[2]; Yvonne Kong[2]; Michelle Cielesh[2]; Youxi Yuan[1]; Atsuko Ito[1]; Benjamin M Eberand[2]; The Huong Chau[3]; Morten Thaysen-Andersen[3]; Freda H Passam[2]; Robert S Haltiwanger[1]; Mark Larance[2]; *[1]Complex Carbohydrate Research Center, Department of Biochemistry and Molecular Biology, University of Georgia, Athens, GA; [2]The University of Sydney, Camperdown, Australia; [3]Macquarie University, North Ryde, Australia*

ThP 372 **Nanoflow liquid chromatography separation to enhance glycopeptide characterization**; David Colquhoun[1]; Patrick Pribil[2]; Jeremy Potriquet[3]; Edward Kerr[4]; Amanda Nouwens[5]; Susan Briscoe[4]; Tony Vuocolo[4]; *[1]Sciex, Framingham, MA; [2]SCIEX, Concord, ON; [3]SCIEX, Mulgrave, Australia; [4]CSIRO, Brisbane, Australia; [5]University of Queensland, Brisbane, Australia*

ThP 373 **Deep sequencing entire glycoproteins with Proteinase K to inform HIV vaccine development**; Sabyasachi Baboo[1]; Jolene K. Diedrich[1]; Jon M Steichen[1]; Torben Schiffner[1]; Kimmo Rantalainen[1]; Olivia Swanson[1]; Christopher A Cottrell[1]; Oleksandr Kalyuzhnyi[1]; Alessia Liguori[1]; William R Schief[1]; James C Paulson[1]; John R. Yates III[1]; *[1]The Scripps Research Institute, La Jolla, CA*

ThP 374 **Fragmentation Featuresof Electronic Excitation Dissociation Tandem Mass Spectra Useful for Accurate Glycosylation Analysis**; Nafisa Tursumamat[1]; Shengyang Liu[1]; Ruiqing Li[1]; Shuhong Guo[1]; Chaoshuang Xia[2]; Joseph Zaia[2]; Catherine E. Costello[2]; Lin Cheng[2]; Juan Wei[1]; *[1]School of Pharmaceutical Sciences, Shanghai Jiao Tong University, Shanghai, China; [2]Center for Biomedical Mass Spectrometry, Boston University Chobanian & Avedisian School of Medicine, Boston, USA, MA*

ThP 375 **Towards MS-based identification and quantification of glycopeptide isomers**; Joshua C.L. Maliepaard[1, 2]; Karli R. Reiding[1, 2]; *[1]Utrecht University, Utrecht, Netherlands; [2]Netherlands Proteomics Center, Utrecht, Netherlands*

ThP 376 **Reversible Enrichment of O-GlcNAcylated Glycopeptides**; Hongqiang Qin; *Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

ThP 377 **Quantitative Evaluation of Affimer and Molecular Imprinted Polymer Affinity Glycoproteins Analysis by Multiple Reaction Monitoring LC-MS/MS**; Billy Molloy[1]; Christian Tiede[2]; Lewis Adams[2]; Darren Tomlinson[2]; Oliver Huseyin[3]; Francesco Canfarotta[4]; Alan Thomson[3]; Johannes Vissers[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]School of Molecular and Cellular Biology, University of Leeds, Leeds, United Kingdom; [3]MIP Discovery, Sharnbrook, United Kingdom; [4]MIP Discovery,, Sharnbrook, United Kingdom*

ThP 378 **In vivo comprehensive profiling of the murine Galnt3-specific O-glycoproteome**; Kruti Dalal[1]; Weiming Yang[1]; E Tian[2]; Aliona Chernish[1]; Peggy McCluggage[1]; Kelly G Ten Hagen[2]; Lawrence A. Tabak[1]; *[1]Biological Chemistry Section, National Institute of Dental and Craniofacial Research, National Institutes of Health, Bethesda, MD; [2]Developmental Glycobiology Section, National Institute of Dental and Craniofacial Research, National Institutes of Health, Bethesda, MD*

ThP 379 **Mass Spectrometry Comparison of N-linked Glycosylation on Influenza A(H3N2) Hemagglutinin in A549 and MDCK Cell lines**; Betlehem Mekonnen[1]; Irina Alymova[2]; Ian York[2]; Dongxia Wang[1]; John R Barr[1]; *[1]CDC, Chamblee, GA; [2]CDC, Atlanta, GA*

ThP 380 **Modifying In Silico Peptide Libraries to Facilitate N-Glycopeptide Real-Time Library Searching**; Kathryn Kothlow[1]; Anna G. Duboff[1]; Jacob H. Russell[1]; Emmajay Sutherland[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle*

ThP 381 **Real-time searching for truncated N-glycopeptides following Endo-H treatment**; Anna G. Duboff[1]; Kathryn Kothlow[1]; Jacob H. Russell[1]; Emmajay Sutherland[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA*

ThP 382 **Expansion of Autonomous-Type Dissociation Selection to Include Core-2 O-Glycopeptides for Improved Characterization of O-Glycopeptides**; Jacob H. Russell[1]; Emmajay Sutherland[1]; Ruby Zhang[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA*

ThP 383 **Comprehensive LC-PAD/MS Analysis of N-glycans using SweetSep™ HPAEC Column**; Christian Marvelous[1]; Jean-Pierre Chervet[1]; Hendrik-Jan Brouwer[1]; Martin Eysberg[2]; Valentina Valentini[2]; *[1]Antec Scientific, Alphen aan den Rijn, Netherlands; [2]Antec Scientific, Boston, MA*

ThP 384 **Veneer is a webtool for rapid, standardized, and transparent interpretation, annotation, and reporting of mammalian cell surface N-glycocapture data**; Linda Berg Luecke[1, 2]; Roneldine Mesidor[1]; Jack Littrel[1]; Morgan Carpenter[1]; Melinda Wojtkiewicz[1]; Rebekah L Gundry[1]; *[1]University of Nebraska Medical Center, Omaha, NE; [2]Medical College of Wisconsin, Milwaukee, WI*

ThP 385 **Introducing DIA Glycoproteomics Analysis in FragPipe**; Daniel Polasky[1]; Fengchao Yu[1]; Weiming Yang[2]; Guo Ci Teo[1]; Yan Wang[3]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Section on Biological Chemistry, National Institute of Dental and Craniofacial Research (NIDCR), NIH, Bethesda, MD; [3]Mass Spectrometry Facility, NICDR, NIH, Bethesda, MD*

ThP 386 **Proton Transfer Charge Reduction to Investigate Co-Isolation in Glycoproteomics**; Kayla Markuson[1]; Ruby Zhang[1]; Nicholas M. Riley[1]; *[1]University of Washington, Seattle, WA*

ThP 387 **N-Glycoproteome of Brain Tissue from the Frontal Lobe is Altered During the Development and Progression of Parkinson's Disease**; Oluwatosin E Daramola[1]; Judith Nwaiwu[2]; Joy Solomon[2]; Moyinoluwa Adeniyi[2]; Andrew I. Bennett[2]; Yehia Mechref[2]; *[1]Texas Tech University, Lubbock, TX; [2]Texas Tech University, Lubbock, Texas*

ThP 388 **Exploring N-glycoproteome characterization with the Orbitrap Astral Mass Spectrometer**; Annie Jen[1]; Noah M. Lancaster[1, 2]; Katherine A. Overmyer[1, 3, 4]; Scott T. Quarmby[1]; Daniel A. Polasky[5]; Alexey I. Nesvizhskii[5]; Joshua J. Coon[1, 2, 3, 4]; *[1]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Morgridge Institute for Research, Madison, WI; [4]National Center for Quantitative Biology of Complex Systems, Madison, WI; [5]University of Michigan, Ann Arbor, MI*

ThP 389 **Isomeric Separation of O-Glycopeptides and Glycosylated Isoforms from Standard Glycoproteins Utilizing Mesoporous Graphitic Carbon (MGC) Material and Tandem MS**; Cristian D Gutierrez-Reyes[1]; Oluwatosin Daramola[2]; Mojibola Fowowe[2]; Sherifdeen B Onigbinde[2]; Judith Ijeoma Nwaiwu[2]; Vishal Sandilya[2]; Yehia Mechref[2]; *[1]Texas Tech University, Lubbock, TX; [2]Texas Tech University, Lubbock, Texas*

ThP 390 **Glycoproteomics of ER-Stress in Cardiomyocytes**; Alexander W Black[1, 2]; Boomathi Pandi[1]; Cheyanne Durham[1]; Dominic C.M. Ng[1]; Maggie P.Y. Lam[1, 2, 3]; *[1]Department of Medicine/Division of Cardiology, University of Colorado School of Medicine, Aurora, CO; [2]Department of Biochemistry and Molecular Genetics, Aurora, CO; [3]Consortium for Fibrosis Research and Translation (CFReT), Aurora, CO*

ThP 391 **Label-free quantification of serum glycopeptides reveals novel biomarkers for advanced colorectal adenoma**; Gege Xu[1]; Rachel Rice[1]; Maryam Baniasad[1]; Ranjan Dalao-

Bhadra[1]; Itati Hundal[1]; Gregg Czerwieniec[1]; Xin Cong[1]; *[1]InterVenn Biosciences, South San Francisco, CA*

ThP 392 **Reproducible enrichment of N-glycopeptides with HPLC Fractionation**; Rachel Rice[1]; Gege Xu[2]; Hector Huang[2]; Maryam Baniasad[2]; Ranjan Bhadra[2]; Xin Cong[2]; *[1]Intervenn Biosciences, South San Francisco, CA; [2]InterVenn Biosciences, South San Francisco, CA*

ThP 393 **Site-specific analysis of co-occupied N- and O-glycopeptides**; Joann Chongsaritsinsuk[1]; Valentina Rangel-Angarita[1]; Keira E. Mahoney[1]; Stacy A. Malaker[1]; *[1]Yale University, New Haven, CT*

ThP 394 **Glycopeptide Enrichment through an All-biomass Synthesized Carbon Nanofiber Aerogel**; Haoran Zhang[1]; Wenxin Wu[1]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, Wisconsin*

ThP 395 **Exploring Site-Specific Glycosylation of Band 3 Protein in Human and Transgenic Porcine Erythrocytes for Xenotransfusion Comparability**; Jae Ho Kim[1, 2]; Myung Jin Oh[1, 2]; Jong Shin Yoo[1, 2]; Joohyun Shim[3]; Kimyung Choi[3]; Hyun Joo An[1, 2]; *[1]Chungnam National University, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; [3]Optipharm Inc., Cheongju, South Korea*

ThP 396 **Fragment ion triggered Parallel Accumulation SErial Fragmentation stepping for enhanced glycoproteomics data acquisition**; Gad Armony[1]; Michael Krause[2]; Pierre-Olivier Schmit[3]; Dennis Trede[2]; Gary Kruppa[4]; Dirk Lefeber[1, 5]; Alain Van Gool[1]; Hans Wessels[6]; *[1]Translational Metabolic Laboratory, Department of genetics, Radboud University Medical Center, Nijmegen, Netherlands; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Bruker Daltonique S.A., Wissembourg, France; [4]Bruker S.R.O., Brno, Czech Republic; [5]Department of Neurology, Donders Institute for Brain, Cognition, and Behavior, Radboud University Medical Center, Nijmegen, Netherlands; [6]Radboudumc, Nijmegen, Netherlands*

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ThP 397 **Unveiling Complexities: Integration of Ion Mobility and Charge-Detection Mass Spectrometry for the Analysis of Multimeric Complexes**; Kyle Juetten[1]; James Sanders[2]; Michael Marty[2]; Jennifer Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX; [2]University of Arizona, Tucson, AZ*

ThP 398 **Improved Mass Accuracy and Precision for MAM using a New Internally Calibrated High Resolution Orbitrap Mass Detector**; Andrew William Dawdy[1]; Edna A Trujillo[1]; Zhenjiu Liu[1]; Julia Kraegenbring[2]; Catharina Crone[2]; Kai Scheffler[3]; *[1]Pfizer, Chesterfield, MO; [2]Thermo Fisher Scientific GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, Germering, Germany*

ThP 399 **Automating Analysis of 1536-well nano-scale High Throughput Environment (HTE) experiments via acoustic ejection high resolution mass spectrometry**; Neal Liddle[1]; Chang Liu[2]; Nomaan Rezayee[1]; Shane Yost[1]; James Garrafa[1]; Joanna Vo[1]; Fred Manby[1]; Mark Spears[3]; Tom Covey[2]; Hui Zhang[1]; *[1]Iambic Therapeutics, San Diego, CA; [2]SCIEX, Concord, ON; [3]Virscidian, Inc, Cary, NC*

ThP 400 **APCI-MS for the analysis of cultural heritage materials**; Anu Teearu-Ojakäär[1]; Signe Vahur[1]; *[1]University of Tartu, Institute of Chemistry, Tartu, Estonia*

ThP 401 **Evaluation of the NIST library matching quality of mass spectra generated by the GC-HR-TOFMS with Multi-Mode Ionization Source**; Craig Fowler[1]; Scott Pugh[1]; George Tikhonov[1]; Slava Artaev[1]; *[1]LECO, St. Joseph, MI*

ThP 402 **Charting New Paths in Lipidomics: An Evaluation of DDA and DIA on an Astral Mass Spectrometer**; Salma I. Abouelhassan[1]; Katherine A Overmyer[1, 2, 3]; Benton J Anderson[1, 3]; Scott T Quarmby[1, 3]; Joshua J Coon[1, 2, 3, 4]; *[1]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Morgridge Institute for Research, Madison, WI; [3]National Center for Quantitative Biology of Complex Systems, Madison, WI; [4]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

ThP 403 **Identification and Quantitation of Low-MW Dendrimer (10183 Da) in Rat Plasma Using QExactive Mass Spectrometry (QE-MS)**; Gabriel Velazquez[1]; Troy Voelker[2]; Brandon Wilcock[2]; Emily Clement[3]; Rémy Poupot[4]; Cédric-Olivier Turrin[3]; *[1]Aliri Bioanalysis, Millcreek, UT; [2]Aliri Bioanalysis, Salt Lake City, UT; [3]IMD-Pharma, Toulouse, France; [4]Université de Toulouse, Toulouse, France*

ThP 404 **Development of the high sensitivity and high resolution post processing methods for biopharmaceutical analyses with multi-turn TOF-MS**; Yusuke Tateishi[1]; Hiroko Morinaga[1]; Hiroyuki Miura[1]; Koichi Kimura[1]; Masaru Nishiguchi[1]; Atsuhiko Toyama[1]; Osamu Furuhashi[1]; Daisuke Okumura[1]; Tairo Ogura[2]; Yuki Yamaguchi[3]; Susumu Uchiyama[3]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Scientific Instruments, Columbia, MD; [3]Osaka university, Osaka, Japan*

ThP 405 **Intercomparison Study of two High-Resolution TOF-MS for Ultra-Trace Detection**; Lena Marie Mokros[1]; Niklas Pengemann[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

ThP 406 **Maximizing the output in metabolomics - Combining high-speed DDA and MRM for simultaneous absolute quantification and non-targeted screening**; Lisa Panzenboeck[1, 2]; Harald Schoeny[1]; Bruno Stelzer[1]; Elisabeth Foels[1, 2]; Marlene Puehringer[1, 2]; Dorian Hirschmann[3]; Christian Dorfer[3]; Daniela Loetsch[3]; Gunda Koellensperger[1, 4]; *[1]Department of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria; [2]Vienna Doctoral School in Chemistry (DoSChem), University of Vienna, Vienna, Austria; [3]Department of Neurosurgery, Medical University Vienna, Vienna, Austria; [4]Vienna Metabolomics Center (VIME), University of Vienna, Vienna, Austria*

ThP 407 **High Resolution Ion Mobility and Ultra-High resolution mass spectrometry for DOM chemical Formula based Structural Assignment**; Pablo R B Oliveira[1]; Dennys Leyva[1]; Lilian V Tose[1]; Muhammad U Tariq[1]; Chad Weisbrod[2]; Fahad Saeed[1]; Francisco A Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]National High Magnetic Field Laboratory, Tallahassee, FL*

ThP 408 **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 409 **INTEGRATION OF TANDEM HIGH RESOLUTION ION MOBILITY AND MASS SPECTROMETRY FOR COMPLEX MIXTURE ANALYSIS**; Andrew R Forero[1]; Miguel Santos[1]; Pablo R B Oliveira[1]; Kevin J. De Fouque[1]; Cullen Greer[2]; Brian H Clowers[2]; Anton N. Kozhinov[3]; Yury Tsybin[3]; Chad R Weisbrod[4]; Fahad Saeed[5]; Francisco A Fernandez-Lima[1, 6]; *[1]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [2]Department of Chemistry, Washington State University, Pullman, WA; [3]Spectroswiss, Lausanne, Switzerland; [4]National High Magnetic Field Laboratory, Tallahassee, Florida; [5]Knight Foundation School of Computing and Information Sciences, Florida International University, Miami, FL; [6]Biomolecular Sciences Institute, Florida International University, Miami, FL*

ThP 410 **Characterization of Monoclonal Antibody (mAbs) using Shimadzu Q-TOF LCMS 9030**; Shannie Tay[1]; Max Kosok[1]; *[1]Shimadzu (Asia Pacific), Singapore, Singapore*

ThP 411 **Assessment of High-Resolution DIA Methods and Short Gradients on High-Throughput μPAC Columns for Maximum Proteome Coverage and Quantitative Performance**; Julia Kraegenbring[1]; Dominic G. Hoch[2]; Jeff Op De Beeck[3]; Riccardo Stucchi[2]; Hanno Resemann[1]; Robert Van Ling[3]; Heiner Koch[1]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Thermo Fisher Scientific, Reinach, Switzerland; [3]Thermo Fisher Scientific, Ghent, Belgium*

ThP 412 **From Rough Signal to Polished Spectrum: Absorption Mode Two-dimensional Mass Spectrometry**; Maria Van

Agthoven[1]; Sarah V Heel[2]; Marek Polak[3, 4]; Alan Kadek[3]; Petr Novak[3, 4]; Kathrin Breuker[2]; Carlos Afonso[1]; Marc-André Delsuc[5]; *[1]University of Rouen-Normandy, Mont-Saint-Aignan, France; [2]University of Innsbruck, Innsbruck, Austria; [3]BioCeV – Institute of Microbiology, The Czech Academy of Sciences, Prague, Czech Republic; [4]Charles University, Prague, Czech Republic; [5]IGBMC Gie CERBM, ILLKIRCH CEDEX, France*

ThP 413 **Advances in Absorption Mode FT-ICR Mass Spectral Quality with MagLab Predator Data Acquisition and Analysis Software**; Greg T Blakney[1]; Amy M McKenna[1]; Chad R Weisbrod[1]; Steve C. Beu[2]; Christopher L Hendrickson[1]; *[1]National High Magnetic Field Laboratory, Tallahassee, Florida; [2]S C Beu Consulting, Austin, TX*

ThP 414 **Metaproteomics optimization on Thermo Astral and Fusion mass spectrometers**; Matthew McIlvin[1]; Paloma Lopez[1]; Mak Saito[1]; *[1]Woods Hole Oceanographic Inst., Woods Hole, MA*

ThP 415 **Capillary Electrophoresis with Absorption Mode Fourier Transform Ion Cyclotron Resonance**; Jonathan Choi[1]; Jon Amster[1]; *[1]University of Georgia, Athens, GA*

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ThP 416 **Metabolite-preserving single cell MALDI imaging reveals metabolite markers of microglia activation in tissue**; James Lucas Cairns[1, 2]; Johanna Huber[1]; Stefan Maurer[3]; Andrea Lewen[4]; Jessica Jung[5]; Stefan Schmidt[1]; Janne Jasmin Wiedmann[6]; Tobias Bausbacher[1]; Pavel Levkin[6, 7]; Philipp Koch[5, 8]; Kerstin Göpfrich[3, 9]; Oliver Kann[4, 10]; Carsten Hopf[1, 2, 5]; *[1]CeMOS, Bioanalytics, University of Applied Sciences Mannheim, Mannheim, Germany; [2]Medical Faculty, Heidelberg University, Heidelberg, Germany; [3]Biophysical Engineering Group, Max Planck Institute for Medical Research, Heidelberg, Germany; [4]Institute of Physiology and Pathophysiology, University of Heidelberg, Heidelberg, Germany; [5]Mannheim Center for Translational Neuroscience (MCTN),, Mannheim, Germany; [6]Institute of Biological and Chemical Systems (IBCS-FMS), Karlsruhe, Germany; [7]Institute of Organic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany; [8]German Cancer Research Center, Heidelberg, Heidelberg, Germany; [9]Biophysical Engineering Group, Center for Molecular Biology of Heidelberg University (ZMBH), Heidelberg, Germany; [10]Interdisciplinary Center for Neurosciences (IZN), Heidelberg, Germany*

ThP 417 **A Machine Learning Approach to System Suitability Testing for Mass Spectrometry Imaging**; Russell R Kibbe[1]; Alexandria L. Sohn[1]; David C. Muddiman[1]; *[1]North Carolina State University, Raleigh, NC*

ThP 418 **Analysis of MSI data using rr2-NMF reveals detailed spectral and spatial visualization of co-localized molecules, both highly and lowly abundant**; Melanie Nijs[1]; Etienne Waelkens[1]; Bart De Moor[1]; *[1]KU Leuven, Leuven, Belgium*

ThP 419 **A technology-neutral software package for integrated spatial multi omics visualization and data analysis**; Nathan Heath Patterson[1]; Wanqiu Zhang[1]; Maria José Q Mantas[1]; Phuong Thao Tran[1]; Reza R Choubeh[1]; Baruch Berger[1]; Fang Xue[2]; M. Reid Groseclose[2]; Pedro Machado Almeida[3]; Alice Ly[1]; Peter Roelants[1]; Thomas Moerman[1]; Nico Verbeeck[1]; Marc Claesen[1]; *[1]Aspect Analytics, Genk, Belgium; [2]GSK, Collegeville, PA; [3]Lunaphore Technologies SA,, Tolochenaz, Switzerland*

ThP 420 **Strategies for assessing and monitoring consistent quality in MALDI Imaging experiments**; Tanja Bien[1]; Ulrike Schweiger Hufnagel[1]; Arne Fuetterer[1]; Hauke Mönck[1]; Stefan Harsdorf[1]; Sergio Legaz[1]; Christoph Nordmann[1]; Corinna Henkel[1]; Janina Oetjen[1]; Nadine T. Smit[1]; Jan H. Kobarg[1]; Matthew R Lewis[2]; Michael Easterling[3]; *[1]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; [2]Bruker UK Limited, Life Sciences Mass Spectrometry Division, Coventry, United Kingdom; [3]Bruker Scientific, 40 Manning Road, Billerica, MA*

ThP 421 **Integrated MALDI-2 MS Imaging and Single-Cell Analysis for Brain Region-Specific Chemical Profiling in Alzheimer's Disease**; Timothy J Trinklein[1]; Stanislav S Rubakhin[1]; Marisa Asadian[1]; K.R. Rajesh[2]; Orly Lazarov[2]; Fan Lam[1]; Jonathan V Sweedler[1]; *[1]University of Illinois Urbana Champaign, Champaign, IL; [2]University of Illinois at Chicago, Chicago, IL*

ThP 422 **Integration and joint multivariate analysis of multimodal chemical imaging data on an example case of hepatocellular carcinoma in rat**; Katharina Kronenberg[1]; Soeren-Oliver Deininger[2]; Marten Seeba[3]; Julia Werner[4]; Peter Bohrer[4]; Rickmer F Braren[4]; Fabian K Lohöfer[4]; Heiko Neuweger[2]; Uwe Karst[1]; *[1]University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [3]Bruker Optics GmbH & Co. KG, Ettlingen, Germany; [4]Institute of Diagnostic and Interventional Radiology, School of Medicine, Technical University of Munich, Munich, Germany*

ThP 423 **Automated Isotope Detection in Imaging Mass Spectrometry Through Spatial and Spectral Cues**; Meenakshi Meenakshi[1]; Lukasz Migas[1]; Katerina V. Djambazova[2, 3]; Martin Dufresne[2, 4]; Jeffrey M Spraggins[2, 3, 4, 5, 6]; Raf Van De Plas[1, 2, 4]; *[1]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [2]Mass Spectrometry Research Center, Nashville, TN; [3]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN; [5]Department of Chemistry, Vanderbilt University, Nashville, TN; [6]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN*

ThP 424 **Spatial Probabilistic Mapping of Metabolite Ensembles in MALDI Mass Spectrometry Imaging**; Denis Abu Sammour[1, 2]; James L. Cairns[3, 4]; Tobias Boskamp[5, 6]; Christian Marsching[3, 5]; Tobias Kessler[7, 8]; Carina Ramallo Guevara[3]; Verena Panitz[8, 9]; Ahmed Sadik[8, 10]; Jonas Cordes[2, 11]; Stefan Schmidt[3]; Shad A. Mohammed[2, 3]; Miriam F. Rittel[2, 3]; Mirco Friedrich[12, 13]; Michael Platten[12, 13]; Ivo Wolf[2, 11]; Andreas Von Deimling[14]; Christiane A. Opitz[8, 9]; Wolfgang Wick[7, 8]; Carsten Hopf[2, 3, 4]; *[1]Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim University of Applied Sciences, Mannheim, Germany; [2]Institute for Medical Technology, Heidelberg University and Mannheim University of Applied Sciences, Mannheim, Germany; [3]Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim University of Applied Sciences, Mannheim, Germany; [4]Medical Faculty Heidelberg, Heidelberg University, Heidelberg, Germany; [5]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [6]Center for Industrial Mathematics, University of Bremen, Bremen, Germany; [7]Clinical Cooperation Unit Neurooncology, German Cancer Consortium, German Cancer Research Center (DKFZ)), Heidelberg, Germany; [8]German Cancer Research Center (DKFZ), Heidelberg, Division of Metabolic Crosstalk in Cancer and the German Cancer Consortium (DKTK), DKFZ Core Center Heidelberg, Heidelberg, Germany; [9]Department of Neurology and National Center for Tumor Diseases, Heidelberg University Hospital, Heidelberg, Germany; [10]Faculty of Bioscience, Heidelberg University, Heidelberg, Germany; [11]Faculty of Computer Science, Mannheim University of Applied Sciences, Mannheim, Germany; [12]Department of Neurology, MCTN, Medical Faculty Mannheim, Heidelberg University, Mannheim, Germany; [13]DKTK Clinical Cooperation Unit Neuroimmunology and Brain Tumor Immunology, DKFZ, Heidelberg, Germany; [14]Department of Neuropathology, University Hospital Heidelberg, and, Clinical Cooperation Unit Neuropathology, German Cancer Research Center (DKFZ), German Cancer Consortium, Heidelberg, Germany*

ThP 425 **Qu-Cee: An Automated Quality Control Pipeline for Cohort and 3-D Imaging Mass Spectrometry**; Lukasz Migas[1]; Ólöf G. Ísberg[2, 3]; David M. G. Anderson[2]; Katerina V Djambazova[2, 3]; Martin Dufresne[2]; Madeline E Colley[2, 4]; Ali Zahraei[2, 3]; Jeffrey M Spraggins[2, 3, 4, 5]; Raf Van De Plas[1, 2, 4]; *[1]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN; [5]Department of Chemistry, Vanderbilt University, Nashville, TN*

ThP 426 **Pyxis Unveiled: Advancing Single-Cell MALDI MSI Analysis for Deeper Molecular Insights**; Ismael Zamora[1]; Rachelle Balez[2]; Jayden C. McKinnon[2]; Reuben S.E. Young[2]; Liam Robinson[2]; Lezanne Ooi[2]; Giuseppe Arturi[3]; Giulia Sorbi[3]; Shane Ellis[2]; Sara Tortorella[3]; *[1]Mass Analytica, S.L, Sant Cugat del Vallés, Spain; [2]Molecular Horizons, University of Wollongong, Wollongong, Australia; [3]Mass Analytica, S.L, Bettona, Italy*

ThP 427 **Measuring Metabolic Fluxes Spatially in Tissues by using Mass Spectrometry Imaging**; Kevin Cho[1]; Michaela Schwaiger-Haber[2]; Ethan Stancliffe[2, 3]; Dhanalakshmi S Anbukumar[2]; Kayla Adkins-Travis[2]; Leah P. Shriver[2]; Gary J. Patti[2]; *[1]Washington University School of Medicine, St. Louis, MO; [2]Washington University in Saint Louis, St. Louis, MO; [3]Panome Bio, Saint Louis, MO*

ThP 428 **imzML Analyzer - open source Python tool for rapid evaluation of MS imaging data: Application to ecotoxicological model Dreissena bugensis**; Matthias Ochs[1]; Nils Weidner[1]; Andreas Roempp[1]; *[1]Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany*

ThP 429 **MS Imaging Spectrum Annotation Tool using Accurate Mass and Isotope Pattern Analysis**; Jeff Dahl[1]; Toshiya Matsubara[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

ThP 430 **Unsupervised co-registration of H&E microscopic images and mass spectrometry images (MSI) with neural networks**; Sai Srikanth Lakkimsetty; *Northeastern University, Boston, MA*

ThP 431 **Assessing Deep Learning Embeddings for MALDI Colocalization**; Lalin Theverapperuma[1]; Leiver Campeon[1]; Nicolas Narvaez Olaya[1]; Pasindu Tennakoon[1]; Andi Krupke[1]; *[1]Expert Intelligence, Santa Clara, CA*

ThP 432 **Artificial Intelligence Tools for Comprehensive 3D Molecular Mapping of Microglia in Mouse Brain Using Mass Spectrometry Imaging**; Aditya Kangune[1]; Connor H Beveridge[2]; Matthew Muhoberac[2]; Jason Finley[2]; Jitika Rajpoot[2]; Palak Manchanda[2]; Lixue Jiang[2]; Emerson Hernly[2]; Julia Laskin[2]; Gaurav Chopra[2, 3, 4, 5, 6, 7, 8]; *[1]Purdue University, Department of Statistics, West Lafayette, IN; [2]Department of Chemistry, Purdue University, West Lafayette, IN; [3]Department of Computer Science (by courtesy), Purdue University, West Lafayette, IN; [4]Purdue Institute for Drug Discovery, West Lafayette, IN; [5]Regenstrief Center for Healthcare Engineering, West Lafayette, IN; [6]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN; [7]Purdue Institute for Inflammation, Immunology, and Infectious Disease, West Lafayette, IN; [8]Purdue Institute for Integrative Neuroscience, West Lafayette, IN*

IMAGING MS: DISEASE MARKERS
433-445

ThP 433 **Exploring cutaneous melanoma through spatially-resolved metabolomics via mass spectrometry imaging and machine learning algorithms**; Yu-Hsuan Chen[1]; Laura Min Xuan Chai[1]; Jia-Fang Tsai[2]; Yi-Hua Liao[2]; Cheng-Chih Hsu[1, 3]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]Department of Dermatology, National Taiwan University, Taipei, Taiwan; [3]Leeuwenhoek Laboratories, Co. Ltd., Taipei, Taiwan*

ThP 434 **Spatial mapping of sulfur-containing metabolites in a mouse model of systemic Staphylococcus aureusinfection**; Justin Ellenburg[1]; Cristina Kraemer-Zimpel[2]; Paige Kies[2]; Neal D Hammer[2]; Boone M. Prentice[1]; *[1]University of Florida, GAINESVILLE, FL; [2]Michigan State University, East Lansing, MI*

ThP 435 **MALDI-MSI Visualization of Cardiolipin Alteration in Rat Organ Tissues after Acute and Chronic Oxidative Stress**; Hay-Yan J. Wang[1]; Chih Le Liu[1]; Ping-Ju Tsai[2]; Kuo-Chen Hung[3]; *[1]Department of Biological Sciences, National Sun Yat-Sen University, Kaohsiung City, Taiwan; [2]Department of Surgery, Yuan's General Hospital, Kaohsiung City, Taiwan; [3]Division of General and Digestive Surgery, Kaohsiung Medical University Chung-Ho Memorial Hospital, Kaohsiung City, Taiwan*

ThP 436 **Utilizing mass spectrometry imaging to identify potential N-glycan prognostic biomarkers for Temozolomide resistance in Glioblastoma Multiforme tissues**; Aaron Angerstein[1]; Lynsday E.A. Young[1]; Xueqing Lun[2]; Grace Grimsley[1]; Donna L Senger[2, 3, 4, 5]; Sabine Hombach-Klonisch[6, 7]; Thomas Klonisch[6, 7, 8]; Richard R Drake[1]; *[1]Medical University of South Carolina, Charleston, SC; [2]Arnie Charbonneau Cancer Institute, Cumming School of Medicine, University of Calgary, Calgary, AB; [3]Department of Oncology, Cumming School of Medicine, University of Calgary, Calgary, AB; [4]Gerald Bronfman Department of Oncology, McGill University, Montreal, QC; [5]Lady Davis Institute for Medical Research, Montreal, QC; [6]Human Anatomy and Cell Science, University of Manitoba, Winnipeg, MB; [7]Pathology, University of Manitoba, Rady Faculty of Health Sciences, Max Rady College of Medicine, Winnipeg, MB; [8]CancerCare Manitoba Research Institute, Winnipeg, MB*

ThP 437 **Multimodal MSI and computational analysis of single amyloid beta (Aβ) plaques reveals Aβ peptide and lipid profiles in Alzheimer's pathology**; Elisabeth Müller[1, 2]; Thomas Enzlein[1]; Carsten Hopf[1, 2]; *[1]Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), University of Applied Sciences Mannheim, Mannheim, Germany; [2]Medical Faculty, Heidelberg University, Heidelberg, Germany*

ThP 438 **Metabolic and Lipidomic Alterations in STZ-Induced Diabetic Mouse Kidneys Revealed Using nano-DESI Mass Spectrometry Imaging**; Syeda Nazifa Wali[1]; Manxi Yang[1]; Frederick Nguele Meke[2]; Zhong-Yin Zhang[2]; Julia Laskin[1]; *[1]Purdue University, Department of Chemistry, West Lafayette, IN; [2]Purdue University, Department of Medicinal Chemistry and Molecular Pharmacology, West Lafayette, IN*

ThP 439 **Mouse model of breast tumor progression shows specific lipid signals linked to Cyp27b1 ablation in the mammary epithelium**; Mengdi Xing[1]; Ethan Yang[2]; Jiarong Li[1]; Ami Grunbaum[1]; Pierre Chaurand[2]; Richard Kremer[1]; *[1]McGill University, Montreal, QC; [2]University of Montreal, Montreal, QC*

ThP 440 **Application of MALDI-MSI to identify and visualize inflammatory mediators in a thermal burn pig skin model**; David Beaver[1]; Celeste C. Finnerty[1]; Andrzej Kudlicki[1]; Brendan Prideaux[1]; *[1]University of Texas Medical Branch at Galveston, Galveston, TX*

ThP 441 **Isotope Encoded Spatial Biology identifies Alzheimer Pathology induced Synaptotoxicity in Space and Time**; Jorg Hanrieder; *University of Gothenburg, Mölndal, Sweden*

ThP 442 **ToF-SIMS imaging reveals changes in tumor cell lipids during metastatic progression of melanoma**; Noora Neittaanmäki[1]; Oscar Zaar[2]; Kevin Sjögren Cehajic[1]; Kelly Dimovska Nilsson[1]; Dimitrios Katsarelias[2]; Roger Olofsson Bagge[1]; John Paoli[1]; John Fletcher[1]; *[1]University of Gothenburg, Gothenburg, Sweden; [2]Sahlgrenska University Hospital, Gothenburg, Sweden*

ThP 443 **Long-Term Lipidomic Changes After Traumatic Brain Injury Using Desorption Electrospray Ionization - Cyclic Ion Mobility Spectrometry - Mass Spectrometry Imaging**; Ludovic Muller[1]; Nivedita Hegdekar[2]; Chinmoy Sarkar[2];

Marta M. Lipinski[2]; Maureen A. Kane[1]; *[1]University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD; [2]University of Maryland, School of Medicine, Department of Anesthesiology, Baltimore, MD*

ThP 444 **Analysis of Metabolite Distribution in Rat Liver of High-Fat Model by Mass Spectrometry Imaging**; Hongmei Mao[1]; Wenjun Wang[2]; Xuesong Xiang[1]; Yan Li[1]; Jinpeng Zhao[1]; Yin Huang[3]; Shuangshuang Di[4, 5]; Qin Zhuo[1]; Honggang Nie[4, 5]; *[1]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; [2]Beijing Junfeix Technology Co., Ltd, Beijing, China; [3]Suzhou PANOMIX Biomedical Technology Co., Ltd, Suzhou, China; [4]Beijing National Laboratory for Molecular Sciences, Peking University, Beijing, China; [5]Analytical Instrumentation Center, Peking University, Beijing, China*

ThP 445 **Dissecting immunometabolism of delta-sarcoglycan deficient hamster model with multimodal mass spectrometry imaging**; Maiko Okamura[1]; Shinichi Yamaguchi[2]; Takushi Yamamoto[2]; Koji Okuda[2]; Shuji Yamashita[3]; Kisaki Amemiya[4]; Kenji Minatoya[5]; Hidetoshi Masumoto[6]; Satoru Noguchi[7]; Ichizo Nishino[8]; Hatsue Ueda[9, 10]; Masaya Ikegawa[3]; *[1]Department of Life and Medical Systems, Doshisha University, Kyotanabe-city, Japan; [2]Shimadzu Corporation, Nakagyo-ku, Japan; [3]Doshisha University, Kyotanabe-city, Japan; [4]Department of Pathology, National Cerebral and Cardiovascular Center, Suita-city, Japan; [5]Department of Cardiovascular Surgery, Graduate School of Medicine, Kyoto University, Sakyo-ku, Japan; [6]Graduate School of Medicine, Kyoto University, Sakyo-ku, Japan; [7]Department of Neuromuscular Research, National Center of Neurology and Psychiatry, Kodaira-city, Japan; [8]National Center of Neurology and Psychiatry, Kodaira-city, Japan; [9]National Cerebral and Cardiovascular Center, Suita-city, Japan; [10]Department of Diagnostic Pathology, Hokusetsu General Hospital, Takatsuki-city, Japan*

IMAGING MS: METHOD DEVELOPMENT II
446-479

ThP 446 **Developing an expansion mass spectrometry (ExMS) method to view the (sub)cellular localization of metabolites in single cells**; Jason A Guerrero[1]; Vignesh Venkataramani[2]; Cole Reinholt[2]; Lydia Kisley[2]; Laura M Sanchez[1]; *[1]University of California, Santa Cruz, Santa Cruz, CA; [2]Case Western Reserve University, Cleveland, Ohio*

ThP 447 **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 448 **Oversampling to Achieve Enhanced Spatial Resolution of Zebrafish by Top-Hat IR-MALDESI-MSI**; Alexandria L. Sohn[1]; Morgan M. Ritter[1]; Seth W. Kullman[1]; Andrew P. Bowman[2]; David C. Muddiman[1]; *[1]North Carolina State University, Raleigh, NC; [2]AbbVie, North Chicago, IL*

ThP 449 **Filter-Assisted Sample Preparation of Liver Organoids for Mass Spectrometry Imaging**; Sohee Yoon[1]; Ahreum Baek[1]; *[1]Korea Research Institute of Standards and Science, Daejeon, South Korea*

ThP 450 **Optimization of human eye cryosectioning for biomarker discovery using mass spectrometry imaging**; Junhai Yang[1]; Andrew P. Bowman[1]; Geraint Parfitt[1]; David Wagner[1]; *[1]AbbVie, North Chicago, IL*

ThP 451 **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[1]; Hsin-Hsiang Chung[1]; Cheng-Chih Hsu[1, 2]; *[1]National Taiwan University, Taipei City, Taiwan; [2]Leeuwenhoek Laboratories, Co. Ltd., Taipei, Taiwan*

ThP 452 **Spatiotemporal lipidomic and proteomic landscape of atherosclerotic plaques in hyperlipidemic mice using imaging mass spectrometry**; ROBIN JOSHI[1]; Soon Yew Tang[1]; E. James Petersson[1]; Garret A. FitzGerald[1]; *[1]University of Pennsylvania, Philadelphia, PA*

ThP 453 **Enhancing Tandem Mass Spectrometry Imaging with De-Mosaicking for Multiplexed Lipid Maps on Tissues**; Aolei Tan[1]; Zheng Ouyang[1]; Xiaoxiao Ma[1]; *[1]Tsinghua University, Beijing, China*

ThP 454 **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[1]; Kaoru Nakagawa[2]; Kenta Terashima[2]; Manami Kobayashi[2]; *[1]Kobe University, Kobe, Japan; [2]Shimadzu Corporation, Nakagyo-ku, Japan*

ThP 455 **Desium: Spatial Transcriptomics and Metabolomics on Single Human Cancer Tissue Sections with DESI-MSI and Visium Spatial Transcriptomics**; Trevor M. Godfrey[1]; Yasmin Shanneik[1]; Faith Jackobs[1]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Houston, TX*

ThP 456 **MALDI mass spectrometry imaging in oriented Caenorhabditis elegans sections**; Ryutaro Jacobson[1]; Elizabeth W. Smith[2]; Yasuaki Saito[1, 3]; Tian Autumn Qiu[1]; *[1]Michigan State University Department of Chemistry, East Lansing, MI; [2]Department of Chemistry, Allegheny College, Meadville, PA; [3]School of Pharmacy, Kitasato University, Shirokane, Minato, Japan*

ThP 457 **Comparing three different ways of oocyte washing before MALDI IMS analysis of lipids**; Paulina Kret[1]; Anna Bodzon-Kulakowska[1]; Przemyslaw Mielczarek[1]; Dominika Siekierska[2]; Wieslawa Mlodawska[2]; Piotr Suder[1]; *[1]AGH University of Krakow, Kraków, Poland; [2]University of Agriculture, Cracow, Poland*

ThP 458 **A workflow for visualizing and annotating oxidized lipids in mass spectrometry imaging analyses**; Kisurb Choe[1]; Lia Tesfay[2]; Jennifer Kyle[1]; Josie G Eder[1]; Theodore Alexandrov[3]; Maria Fedorova[4]; Suzy Torti[2]; Christopher Robert Anderton[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of Connecticut, Storrs, CT; [3]EMBL, Heidelberg, Germany; [4]Dresden University of Technology, Dresden, Germany*

ThP 459 **prmImaging: an integrated workflow for the analysis and interpretation of spatial on-tissue tandem mass spectrometry of lipids**; Nannan Tao[1]; Bram Heijs[2]; Tobias Boskamp[2]; Soeren-Oliver Deininger[2]; Nikolas Kessler[2]; Arne Fuetterer[2]; Arne Behrens[2]; Corinna Henkel[2]; Nadine T. Smit[2]; Katherine Stumpo[3]; *[1]Bruker Daltonics Inc., Billerica, MA; [2]Bruker Daltonics, Bremen, Germany; [3]Bruker Daltonics, Billerica, MA*

ThP 460 **Deep molecular coverage at faster throughput: IR Guided MALDI Imaging in cancer research**; Arne Behrens[1]; Domenic Dreisbach[2]; Ethan Yang[3]; Peng Wang[4]; Annika Nyhuis[1]; Soeren-Oliver Deininger[1]; Joshua L. Fischer[3]; Azad Eshghi[3]; Hans-Christian Koch[2]; *[1]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [2]Bruker Optics GmbH & Co. KG, Ettlingen, Germany; [3]Bruker Scientific, 40 Manning Road, Billerica, MA; [4]Bruker Optics LLC, Billerica, MS*

ThP 461 **Hyperplex MALDI-IHC Proteomics Imaging Reveals the Heterogeneity of Endometrial Cancer Spatial Structure**; Mengze Zhang[1, 2]; John Abbey[2, 3]; Pierre Bost[4]; Mark J. Lim[5]; Gargey B. Yagnik[5]; Andrew Yatsuhashi[5]; Kenneth J. Rothschild[5, 6]; Bernd Bodenmiller[2, 3]; *[1]University of Zurich, Zurich, Switzerland; [2]ETH Zurich, Zurich, Switzerland; [3]University of Zurich, Zürich, Switzerland; [4]Institut Curie, PSL University, Sorbonne Université, Paris, France; [5]AmberGen Inc., Billerica, MA; [6]Boston University, Department of Physics and Photonics Center, Boston, MA*

ThP 462 **Single-cell Multiplexed Imaging and Profiling with Fluorescence-Ion Microscopy (FIM)**; Yuchen Xiang[1]; Daniel Simon[1]; Stefania Maneta-Stavrakaki[1]; Zoltan Takats[1]; *[1]Imperial College London, London, United Kingdom*

ThP 463 **Expansion Imaging Mass Spectrometry for High Spatial Resolution Lipid Analysis using a Superabsorbant Hydrogel**; Jacob M Samuel[1]; Tingting Yan[2]; Boone M.

Prentice[2]; *[1]University of Florida Department of Chemistry, Gainesville, FL; [2]University of Florida, Chemistry Department, Analytical Chemistry Division, Gainesville, FL*

ThP 464 **Targeted protein imaging of kidney pathologies using MALDI Imaging**; Katherine A. Stumpo[1]; Corinna Henkel[2]; Taylor Skurnac[1]; Jessica Schmitz[3]; Jan Hinrich Braesen[3]; *[1]Bruker Scientific, 40 Manning Road, Billerica, MA; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [3]Nephropathology Unit, Institute for Pathology, Hannover Medical School, Hannover, Germany*

ThP 465 **Light-Activated Derivatization of Lipids for Isomer Analysis by MALDI Mass Spectrometry**; Thomas R Fredriksen[1]; Joseph H Holbrook[2]; Ana L. Mora[3]; Mauricio Rojas[4]; Amanda B Hummon[5, 6]; *[1]The Ohio State University, Columbus, OH; [2]The Ohio State Biochemistry Program, Columbus, Ohio; [3]The Ohio State University Department of Internal Medicine Division of Pulmonary, Critical Care & Sleep Medicine, Columbus, Ohio; [4]The Ohio State University Department of Internal Medicine, Columbus, Ohio; [5]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, Ohio; [6]Comprehensive Cancer Center, The Ohio State University, Columbus, OH, 43210*

ThP 466 **Addition of Heavy Metal Detection to the MALDI IMS Repertoire for Simultaneous Imaging of Exogenous Metals and Endogenous Bioanalytes**; Kes A Luchini[1]; Tara Harvey[2, 3]; Grace M. Thornhill[2, 3]; Abigale S Mikolitis[2, 3]; Zachary J. Sasiene[2, 3]; Joshua D. Breidenbach[2, 3]; Ethan M. McBride[2, 3]; Brett R. Blackwell[2, 3]; Austin R. Anderson[2, 3]; Lauren K. Heine[2, 3]; Chi-Yen Tseng[2, 3]; Jessica A. Salguero[2, 3]; Francisca E. Rodriguez[2, 3]; Salvator J. Palmisano[2, 3]; Erick S. LeBrun[2, 3]; Phillip M. Mach[2, 3]; Trevor G. Glaros[2, 3]; Emilio S. Rivera[2, 3]; *[1]Los Alamos National Laboratory, Los Alamos, NM; [2]Mass Spectrometry Center for Integrated Omics, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM; [3]Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM*

ThP 467 **Cellular-level resolution DESI-MS imaging**; Chengyi XIE[1, 2]; Jianing WANG[1, 2]; Zongwei CAI[1, 2]; *[1]State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Kowloon Tong, Kowloon, China; [2]Department of Chemistry, Hong Kong Baptist University, Kowloon Tong, Kowloon, China*

ThP 468 **Submicron Resolution MALDI Mass Spectrometry Imaging of Lipids at the Subcellular Level**; Chengyi Xie[1, 2]; Jianing Wang[1]; Zongwei Cai[1, 2]; *[1]State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, China; [2]Department of Chemistry, Hong Kong Baptist University, Kowloon Tong, Kowloon, China*

ThP 469 **Molecular profiling of glioblastoma patient-derived single cells using combined MSI and MALDI-IHC**; Kasper K Krestensen[1]; Marleen Derweduwe[2]; Frederik De Smet[2]; Eva Cuypers[1]; Ron Heeren[1]; *[1]M4I Division of Imaging Mass Spectrometry, Maastricht University, Maastricht, Netherlands; [2]KU Leuven, Leuven, Belgium*

ThP 470 **Met-ID: a graphical user interface for rapid MALDI-MSI metabolite identification**; Patrik Bjärterot[1]; Anna Nilsson[1]; Reza Shariatgorji[1]; Theodosia Vallianatou[1]; Ibrahim Kaya[1]; Lukas Käll[2]; Per Svenningsson[3]; Per E. Andrén[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Royal institute of Technology, Stockholm, Sweden; [3]Karolinska Institutet, Stockholm, Sweden*

ThP 471 **Imaging Technologies for Constructing 3D Multimodal Lipid Atlases of the Eye**; David M. G. Anderson[1]; Lukasz Migas[2]; Jeffery Messinger[3]; Raf Van De Plas[2]; Dongfeng N Cao[4]; Richard M. Caprioli[1]; Christine A Curcio[3]; Kevin L. Schey[1]; Jeffrey M Spraggins[5]; *[1]Vanderbilt University, Department of Biochemistry, Nashville, TN; [2]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [3]University of Alabama Birmingham, Birmingham, Alabama; [4]University of Alabama at Birmingham, Birmingham, AL; [5]Vanderbilt University, Nashville, TN*

ThP 472 **Uncovering ferroptotic cells as pathogenic drivers in diseased tissue using Dual-SIMS imaging at 1 µm resolution**; Hua Tian[1]; Kavita Vats[2]; Louis J. Sparvero[1]; Kunal Singh[2]; Yulia Y. Tyurina[1]; Hülya Bayır[3]; Valerian E. Kagan[1]; Yuri L. Bunimovich[2]; *[1]Center for Free Radical and Antioxidant Health, Department of Environmental Health and Occupational Health, University of Pittsburgh, Pittsburgh, PA; [2]Department of Dermatology, University of Pittsburgh School of Medicine, Pittsburgh, PA; [3]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 473 **Enhancing MALDI IMS Sensitivity and Specificity of Neutral Lipids via Salt Doping and Ion Mobility**; Kameron Molloy[1, 2]; Madeline E Colley[2, 3]; Martin Dufresne[2, 3]; Lukasz Migas[2, 4]; Raf Van De Plas[2, 3, 4]; Jeffrey M Spraggins[1, 2, 3, 5, 6]; *[1]Department of Chemistry, Vanderbilt University, Nashville, TN; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [6]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN*

ThP 474 **MALDI-2 Mass Spectrometry Imaging of Peptide Toxins, Lipopeptides and Lipids in Thin Sections of Bacillus subtilis Biofilms**; Kim Lena Wüpping[1]; Jan-Philipp Knepper[1]; Alexander Potthoff[1]; Jens Soltwisch[1]; Klaus Dreisewerd[1]; *[1]Institute of Hygiene, University of Münster, Münster, Germany*

ThP 475 **Image Deconvolution Restores MSI Spatial Resolution Following Signal Averaging**; Yury Desyaterik[1]; Mary Peace McRae[2]; Angela DM Kashuba[1]; Konstantin O. Nagornov[3]; Anton N. Kozhinov[3]; Yury O. Tsybin[3]; Elias P. Rosen[1]; *[1]UNC, Chapel Hill, NC; [2]University of Virginia, Charlottesville, VA; [3]Spectroswiss, Lausanne, Switzerland*

ThP 476 **Lithium doped nanospray desorption electrospray ionization mass spectrometry imaging for enhanced metabolite coverage**; Kiera Nguyen[1]; Nathalie Costie[2]; Gillian Carleton[2, 3]; Tian Zhao[2, 3]; Julian J. Lum[2, 3]; Kyle D Duncan[1, 4]; *[1]Department of Chemistry, Vancouver Island University, Nanaimo, BC; [2]Trev and Joyce Deeley Research Centre, BC Cancer, Victoria, BC; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [4]Department of chemistry, University of Victoria, Victoria, BC*

ThP 477 **MS imaging enabling visualization of lipid C=C positional isomers in biological tissues using Oxygen Attachment Dissociation (OAD)**; Kaoru Nakagawa[1]; Hidenori Takahashi[1]; Satoshi Kasamatsu[1]; Kengo Takeshita[1]; Manami Kobayashi[2]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]SHIMADZU Corporation, Kawasaki, Japan*

ThP 478 **New workflows for 3-D multimodal molecular imaging based on sequential 2-D data**; Ellie L Pingry[1, 2]; Lukasz Migas[3, 4]; David Anderson[1, 5]; Felipe A Moser[4]; Angela R. S. Kruse[1, 2]; Melissa A. Farrow[3, 5]; Raf Van De Plas[1, 4, 5]; Jeffrey M Spraggins[1, 2, 5, 6, 7]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [3]Mass Spectrometry Research Center, Nashville, TN; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Department of Biochemistry, Vanderbilt University, Nashville, TN; [6]Department of Chemistry, Vanderbilt University, Nashville, TN; [7]Department of Pathology, Microbiology and Immunology, Vanderbilt University Medical Center, Nashville, TN*

ThP 479 **Advances in top-down HRMS with AP/MALDI orbitraps for spatial analysis of peptides/metabolites in human**

pathology FFPE tissue archives; Peter D. Verhaert[1]; Gilles Frache[2]; Maureen Feucherolles[2]; Sooraj Baijnath[3]; Aletta Millen[3]; Dick Swaab[4, 4]; Lin Zhang[4]; Cecilia Lindskog[5]; Mathias Uhlén[6]; Marthe Verhaert[7]; Raf Sciot[8]; *[1]ProteoFormiX, Beerse, Belgium; [2]Luxembourg Institute of Science and Technology, Belvaux, Luxembourg; [3]Integrated Molecular Physiology Research Initiative, Johannesburg, South Africa; [4]Netherlands Institute for Neuroscience, Amsterdam, Netherlands; [5]Uppsala university, Uppsala, Sweden; [6]KTH Royal Institute of Techonology, Stockholm, Sweden; [7]BITOX Belgian Immunotoxicity Board, Brussels, Belgium; [8]University Hospitals Leuven, Heverlee, Belgium*

INFORMATICS: GENERAL, SRM, AND DIA
480-487

ThP 480 **DeepRTAlign: toward accurate retention time alignment for large cohort mass spectrometry data analysis**; Yi Liu; *Beijing Proteome Research Center, Beijing, China*

ThP 481 **Using Graphs to Visualize and Simplify Complex Mass Spectra**; Ron Bonner[1]; Gerard Hopfgartner[2]; *[1]Ron Bonner Consulting, Newmarket, ON; [2]University of Geneva, Geneva, Switzerland*

ThP 482 **PepQuery-DIA: Streamlining Fast and Accurate Proteomic Validation of Novel Genomic Alterations Using DIA Data**; Wenrong Chen[1, 2]; Matthew V. Holt[1, 2]; Yu Wen[3]; Jixin Wang[4]; Wenyan Zhong[5]; Bing Zhang[6]; *[1]Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; [2]2Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX; [3]Data Science and AI, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, MD; [4]Oncology Data Science, AstraZeneca, Gaithersburg, MD; [5]Oncology Data Science, Oncology R&D, AstraZeneca, New York, NY; [6]Baylor College of Medicine, Houston, Texas*

ThP 483 **Developing a massive multi-instrument manually curated chromatogram training library**; Brian C. Searle[1]; Ariana E Shannon[1]; Katelyn B Brusach[1]; Regina M Edgington[1]; Gautam Ghosh[1]; Alex W Joyce[1]; Madalyn G Moore[1]; Chase Renzelmann[1]; Damien B Wilburn[1]; *[1]The Ohio State University, Columbus, OH*

ThP 484 **Automated Quality Control Assessment for Large-Scale Proteomics Datasets**; Niveda Sundararaman[1]; Manasa Vegesna[1]; Aleksandra Binek[1]; Jennifer E. Van Eyk[1]; *[1]Cedars Sinai Medical Center, Los Angeles, CA*

ThP 485 **Mass++ ver.4 Gold (official release), an Open-Source MS Data Viewer**; Satoshi Tanaka[1, 2]; Masaki Murase[2]; Masaki Kato[2, 3]; Hiroyuki Yamamoto[2, 4]; Tsuyoshi Tabata[2, 5]; Maiko Kusano[2, 6]; Shin Kawano[2, 7]; Shujiro Okuda[8]; Akiyasu C. Yoshizawa[2, 8]; *[1]Trans-IT, Mibu-machi, Japan; [2]Mass++ Users Group,, Kyoto, Japan; [3]Data Knowledge Organization Unit, RIKEN Information R&D and Strategy Headquarters, RIKEN, Wako, Japan; [4]Human Metabolome Technologies, Inc., Tsuruoka, Japan; [5]Grad. School of Pharma. Sci., Kyoto Univ., Kyoto, Japan; [6]School of Medicine, Showa Univ., Shinagawa, Japan; [7]School of Frontier Engineering, Kitasato Univ., Sagamihara, Japan; [8]Medical AI Center, School of Medicine, Niigata Univ.,, Niigata, Japan*

ThP 486 **Speeding up panel development for targeted proteomics using deep learning: a proof-of-concept based on a prostate cancer study**; Tikira Temu[1]; Oliver M. Bernhardt[1]; Véronique Laforte[1]; Sebastian Mueller[1]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

ThP 487 **Improved library free dia-PASEF based quantitative proteomics using Spectronaut**; Tejas Gandhi[1]; Monika Pepelnjak[1]; Christopher Below[1]; An-phi Nguyen[1]; Véronique Laforte[1]; Roland Bruderer[1]; Oliver M. Bernhardt[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

INFORMATICS: MULTIOMICS INTEGRATION
488-506

ThP 488 **Nonlinear Dynamic Changes During Human Aging Revealed in Multi-omics Profiles**; Xiaotao Shen[1]; Chuchu Wang[1]; Xin Zhou[1]; Wenyu Zhou[1]; Daniel Hornburg[1]; Si Wu[1]; Michael Snyder[1]; *[1]Stanford University, Palo Alto, CA*

ThP 489 **GlycoLibraries: Hybrid-search-based bootstrapping method identifies and annotates oligosaccharides, gangliosides and glycopeptides in complex matrices**; Concepcion Remoroza[1]; Yi Liu[1]; Meghan Burke[1]; Yuxue Liang[1]; Xiaoyu Yang[1]; Tytus Mak[1]; Sergey Sheetlin[1]; Yuri Mirokhin[1]; Dmitrii Tchekhovskoi[1]; Stephen Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

ThP 490 **Protein profiling of zebrafish embryos unmasks a new regulatory layer during early embryogenesis**; Gabriel Da Silva Pescador[1]; Danielson Baia Amaral[1]; Joseph M Varberg[1]; Ying Zhang[1]; Yan Hao[1]; Laurence Florens[1]; Ariel A Bazzini[1, 2]; *[1]Stowers Institute for Medical Research, Kansas City, MO; [2]Department of Molecular and Integrative Physiology, University of Kansas School of Medicine, Lawrence, KS*

ThP 491 **Multi-Omics Data Visualization in BioCyc**; Peter Karp[1]; Austin Swart[1]; Suzanne Paley[1]; *[1]SRI International, Menlo Park, CA*

ThP 492 **Multi-Omics unveils disruption of shared metabolic pathways in Caco-2 Cells and C. elegans exposed to Organophosphate flame retardants.**; Ahn Jeongjun[1]; Kim Hyung Min[2]; Kang Jong Seong[2]; *[1]chungnam national university, daejeon, South Korea; [2]Chungnam National University, Daejeon, South Korea*

ThP 493 **Functional Integrative Enrichment Metric Score for proteomics enrichment analysis**; Maciej Dulewicz[1]; Henrik Zetterberg[1, 2]; Kaj Blennow[1]; Jörg Hanrieder[1, 2]; *[1]University of Gothenburg, Gothenburg, Sweden; [2]Department of Neurodegenerative Disease, UCL Institute of Neurology, London, United Kingdom*

ThP 494 **Proteomic Insights into the Effects of Blueberry and Cranberry Crops on Honey Bee Health and Physiology**; Huan Zhong[1]; Yuming Shi[1]; Jason Rogalski[1]; Renata Moravcova[1]; Leonard Foster[1]; *[1]UBC, Vancouver, BC*

ThP 495 **Multi-omics characterization of anti-CD40 induced mouse colitis model**; Liang Jin[1]; Michael Macoritto[1]; Nikolaus Berndt[2]; Xue Wang[1]; Ruoqi Peng[1]; Annette Schwartz Sterman[1]; Yu Tian[1]; *[1]AbbVie Bioresearch Center, Worcester; [2]Doppelganger Biosystem GmbH, Oldenburg, Germany*

ThP 496 **A multi-scale map of proteome organization from integration of protein interactions and images**; Leah V Schaffer[1]; Mengzhou Hu[1]; Edward L Hutlin[2]; Gege Qian[1]; Abantika Pal[3]; Neelesh Soni[3]; Andrew P Latham[3]; Kyung-Mee Moon[4]; Laura Pontano Vaites[2]; Trang Le[5]; Yue Qin[1]; Dexter Pratt[1]; Christopher Churas[1]; Leonard J Foster[4]; Ignacia Echeverria[3]; J Wade Harper[2]; Steven P. Gygi[2]; Emma Lundberg[5, 6, 7]; Trey Ideker[1]; *[1]University of California, San Diego, San Diego, CA; [2]Harvard Medical School, Boston, MA; [3]University of California-San Francisco, San Francisco, CA; [4]University of British Columbia, Vancouver, BC; [5]Stanford University, Stanford, CA; [6]KTH Royal Institute of Techonology, Stockholm, Sweden; [7]Chan-Zuckerburg Biohub, San Francisco, California*

ThP 497 **M2IA: metabolic pathway-reaction-metabolite-based strategy for advanced integrative analysis of gut microbiome, metabolome, and phenotype**; Yan Ni[1]; Cuifang Xu[1]; *[1]Children's Hospital, Zhejiang University School of Medicine, National Clinical Research Center for Child Health, Hangzhou, China*

ThP 498 **Complete, Precise and Fast Proteogenomic Analysis with pAnno2**; Kaifei Wang[1]; Mingkun Yang[2, 3]; Zhuohong Wei[1]; Feng Ge[2, 3]; Hao Chi[1]; *[1]Key Laboratory of Intelligent Information Processing of Chinese Academy of Sciences (CAS), Institute of Computing Technology, Beijing, China; [2]State Key Laboratory of Freshwater Ecology and Biotechnology, Institute of Hydrobiology, Chinese Academy of Sciences, Wuhan, China; [3]Key Laboratory of Algal Biology, Institute of Hydrobiology, Chinese Academy of Sciences, Wuhan, China*

ThP 499 **Integrated Metabolomics and Proteomics Reveals Systemic and Localized Metabolic Disruptions in Colorectal Cancer**; Ethan Stancliffe[1]; Adam D. Richardson[1];

Monil Gandhi[1]; Ashima Mehta[1]; Kevin Y Cho[2]; Gary J. Patti[1, 2]; *[1]Panome Bio, Saint Louis, MO; [2]Washington University in Saint Louis, St. Louis, MO*

ThP 500 **ShowMEPATH: Automated Multi-Omics Comparative Analysis Tool Unveiling Hidden Patterns in Large-Scale Fold Change Data**; Manhoi Hur[1, 2]; Hee-Seung Choi[1]; Wilhelmina Van De Ven[1]; Katayoon Dehesh[1]; *[1]University of California, Riverside, RIVERSIDE, California; [2]UCR Metabolomics Core, University of California, Riverside, California*

ThP 501 **A systems-scale approach to identifying protein isoforms modulating endothelial cell development**; Madison M Mehlferber[1]; David Wissel[2]; Erin D Jeffery[1]; Vasilii Pavelko[1]; Jennifer A Korchak[1]; Micah Lehe[1]; Marcus J. Meade[1]; Gloria Sheynkman[1]; *[1]University of Virginia, Charlottesville, VA; [2]University of Zurich, Zürich, Switzerland*

ThP 502 **Deep plasma proteomics enables identification of sample-swap issues in a large multi-omics discovery study**; Yuntao Hu[1]; Jinlyung Choi[1]; Ajinkya Kokate[1]; Sara Nouri Golmaei[1]; Daniel Ariad[1]; Ehdieh Khaledian[1]; Guanhua Shu[1]; Purva Ranjan[1]; Manway Liu[1]; Joon-Yong Lee[1]; Bruce Wilcox[1]; Chinmay Belthangady[1]; *[1]Prognomiq Inc., San Mateo, California*

ThP 503 **Unique opportunities in cross-omics analysis of plasma multiomics data using prior knowledge**; Austin Quach[1, 2]; Whitaker Cohn[2]; Rachel Kwan[1]; Olivia Choi[1]; Seungjun Yeo[1]; Julian Whitelegge[2]; *[1]Dalton Bioanalytics Inc., Los Angeles, CA; [2]UCLA Pasarow Mass Spectrometry Laboratory, Los Angeles, CA*

ThP 504 **ProteoImager: an integrative platform for image coregistration, spatial analysis, and visualization for high-resolution spatial proteomics datasets**; Zhenru Zhou[1]; Amanda Lorentzian[1]; Yikai Luo[1]; Zhichang Yang[1]; Anatoly Belov[1]; Melissa Gonzalez[1]; Miriam Baca[1]; James Ziai[1]; Ying Zhu[1]; Meena Choi[1]; *[1]Genentech Inc., South San Francisco, CA*

ThP 505 **Integration of untargeted metabolomics with targeted profiling of inflammatory proteins to define the metabolic fingerprint of inflammation in COVID-19**; Monil Gandhi[1]; Adam Richardson[2]; Ethan Stancliffe[2]; Ashima Mehta[2]; Kevin Y Cho[3]; Gary J. Patti[1, 3]; *[1]PanomeBio, St Louis, MO; [2]Panome Bio, Saint Louis, MO; [3]Washington University in Saint Louis, St. Louis, MO*

ThP 506 **SimpliFi in a Box: multiomics data analysis on private servers**; Jim Palmeri[1]; John P Wilson[1]; *[1]Protifi, LLC, Fairport, NY*

INSTRUMENTATION: NEW CONCEPTS
507-523

ThP 507 **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[1]; Jaskiran Kaur[1]; Ruth O. Anyaeche[1]; Yuyang Zhang[1]; Kawthar Z. Alzarieni[1, 2]; Hendrik M. Ma[1]; Annika M. Little[1]; Tanya Sharma[1]; Matthan D. Nussbaum[1]; Drake A. Hershberger[1]; Ying-jou Lee[1]; Voislav Blagojevic[3]; Justin L. Neill[3]; Hilkka I Kenttämaa[1]; *[1]Purdue University, West Lafayette, IN; [2]Jordan University of Science and Technology, Irbid, Jordan; [3]BrightSpec Inc., Charlottesville, VA*

ThP 508 **Image-Guided Laser Ablation System for Precise 3D Tissue Sampling for Subsequent Analysis of Biomolecules in Cancer Research**; Jan Hahn[1, 2, 3]; Manuela Moritz[1]; Anton Walter[1]; Tamara Wieck[1]; Ayham Moustafa[1]; Marie-Therese Haider[1, 3]; Tobias Lange[1, 4]; Hartmut Schlüter[1, 3]; *[1]University Medical Center Hamburg-Eppendorf (UKE), Hamburg, Germany; [2]Mildred Scheel Cancer Career Center HaTriCS4, Hamburg, Germany; [3]University Cancer Center Hamburg, Hamburg, Germany; [4]University Hospital Jena, Jena, Germany*

ThP 509 **Mass Resolution in PTR-TOFMS: The more, the better?**; Alfons Jordan[1]; Christian Lindinger[1]; Andreas Mauracher[1]; Rene Gutmann[1]; Stefan Feil[1]; Paul Mutschlechner[1]; Todd Rogers[2]; Philipp Sulzer[1]; *[1]IONICON Analytik GmbH., Innsbruck, Austria; [2]Trace VOC, Kennewick, WA*

ThP 510 **A novel technology for sample preparation: A fully automated, high-throughput and online electro-extraction platform hyphenated to LC-MS analysis**; Yupeng He[1]; Paul Miggiels[1]; Nicolas Drouin[1]; Amy C. Harms[1]; Bert Wouters[1]; Thomas Hankemeier[1]; *[1]Leiden University, Leiden, Netherlands*

ThP 511 **Utilizing Charged Residue Mechanism in Electrospray Droplets for Cryo-EM Sample Preparation**; Liwen Liang[1]; Jingjin Fan[1, 2]; Zi Yang[1]; Zheng Pang[1]; Zheng Ouyang[1]; Hong-Wei Wang[1]; Xiaoyu Zhou[1]; *[1]Tsinghua University, Beijing, China; [2]University of Oxford, Oxford, United Kingdom*

ThP 512 **Mobility Selective Ion Soft-Landing Using Structures for Lossless Ion Manipulation (SLIM)**; Sandilya Garimella[1]; Jung Yun Lee[1]; Ailin Li[1]; Prabhakaran Venkateshkumar[1]; Xin Zhang[1]; Harrilal P Christopher[1]; Libor Kovarik[1]; Yehia M Ibrahim[1]; Richard D Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

ThP 513 **A universal design for high-resolution linear time-of-flight mass spectrometers with a wide m/z range**; Yi-Hong Cai[1]; Yi-Sheng Wang[1]; *[1]Genomics Research Center Academia Sinica, Taipei, Taiwan*

ThP 514 **A Functionalized Vacuum Flange to Power Ion Guides, Funnels, and Traps**; Caraleigh G. Smith[1]; Brian H Clowers[2]; Zackary R Kinlein[2]; Steven J Kregel[1]; *[1]Bradley University, Peoria, IL; [2]Washington State University Department of Chemistry, Pullman, WA*

ThP 515 **Exploring sex differences in zebrafish livers using a novel targeted discovery metabolomics approach**; Michaela Schwaiger-Haber[1]; Bashar Amer[2]; Darshak Gadara[1]; Cristina C. Jacob[2]; Philip M. Remes[2]; Susan S. Bird[2]; Gary J. Patti[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 516 **Design and optimization of a band-pass device for a quadrupole ion guide**; Yang Kang[1]; Mircea Guna[1]; David Cox[1]; Andrei Sonoc[1]; Ian Moore[1]; Bradley Schneider[1]; *[1]SCIEX, Concord, ON*

ThP 517 **Analysis of VOCs in aqueous solutions using the coupling of an oven with a mobile FT-ICR-MS associated to chemical ionization**; Taous ABAR[1]; Michel Heninger[1]; Joel Lemaire[1]; Hélène Mestdagh[1]; *[1]Institut de Chimie Physique - Université Paris-Saclay, Orsay, France*

ThP 518 **Streamlining effective translational research using a novel hybrid nominal mass spectrometer acquisition for comprehensive molecular profiling**; Scott Peterman[1]; Scott D Stanley[2]; Abigail Burrows Franco[2]; Phillip Remes[3]; Cristina Jacobs[3]; *[1]Thermo Fisher Scientific, Fort Walton Beach, FL; [2]University of Kentucky, Lexington, KY; [3]Thermo Fisher Scientific, San Jose, CA*

ThP 519 **Transmission Nano-Projectile Secondary Ion Mass Spectrometry - A Method for Accurate Analysis of Nanoparticles**; Michael A. Shaw[1]; Michael J. Eller[1]; *[1]California State University Northridge, Northridge, CA*

ThP 520 **Virtual-Slit Cycloidal Mass Spectrometry of Actinide Particles**; Rafael Bento Serpa[1]; Charles B. Parker[1]; Elizabeth D. LaBone[2]; Christopher Zarzana[3]; Justin Keogh[4]; Jonathon Andrus[3]; Nathan A. Stevens[3]; Rosalie Greer[2]; Kyle M. Samperton[2]; Danielle Mannion[2]; Joe Mannion[2]; Jeffrey T. Glass[1]; M. Bonner Denton[4]; Jason J. Amsden[1]; *[1]Duke University, Durham, NC; [2]Savannah River National Laboratory, Aiken, SC; [3]Idaho National Laboratory, Idaho Falls, ID; [4]University of Arizona, Tucson, AZ*

ThP 521 **Narrowed isolation in the low mass range using a digital QTOF**; Elizabeth Groetsema[1]; Sumeet S. Chakravorty[1]; Fatima Olayemi Obe[1]; Gordon A Anderson[2]; Shane Tichy[3]; Adam P. Huntley[1]; Brian H Clowers[1]; Peter T. A. Reilly[1]; *[1]Washington State University Department of Chemistry, Pullman, WA; [2]GAA Custom Electronics LLC, Kennewick, WA; [3]Agilent Technologies, Santa Clara, CA*

ThP 522 **Practical Quadrupole Theory: Rectilinear Quadrupole and Hexapole Ion Guides Operated with Collisional**

Damping Pressures; Jacob Pasko[1]; Randall E Pedder[1]; Luke Metzler[1]; [1]*Ardara Technologies, Ardara, PA*

ThP 523 **High Dynamic Range Data Acquisition System for TOFMS tools**; Amit Weingarten[1]; Pierre-François Maistre[2]; Aleksey Vorobyev[3]; Vasily Makarov[3]; Anatoly Verenchikov[3]; [1]*El-Mul Technologies, Rehovot, Israel;* [2]*Acqiris SA, Geneva, Switzerland;* [3]*MSC-CG, Bar, Montenegro*

INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING
524-542

ThP 524 **Evaluation of Gas dynamics of source nozzle geometry by simulation and LDTD-MS/MS experiment**; Pierre Picard[1]; Sarah Demers[1]; Jean Lacoursière[1]; Jonathan Rochon[1]; Mégane Moreau[1]; Serge Auger[1]; [1]*Phytronix Technologies, Inc., Quebec, QC*

ThP 525 **Variable Temperature Electrospray Measurement of Enthalpy and Entropy of Tryptophan Binding to Ring Shaped Protein TRAP**; William J Moeller[1, 2]; Mark P Foster[3]; Vicki H Wysocki[2, 3]; [1]*The Ohio State University, Columbus, OH;* [2]*Native Mass Spectrometry Guided Structural Biology Center, The Ohio State University, Columbus, OH;* [3]*Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH*

ThP 526 **Plasma-in-Droplet Ionization Mass Spectrometry**; Dmytro S Kulyk[1]; Purva S. Damale[1]; Abraham K. Badu-Tawiah[1]; [1]*OSU, Columbus, OH*

ThP 527 **Triboelectric Nanogenerator-Coated Blade Spray Mass Spectrometry (TENG-CBS MS) for Volume-limited Drug Analysis**; Xin Ma[1]; Facundo M. Fernández[1, 2]; [1]*School of Chemistry and Biochemistry, Georgia Institute of Technology, Altanta, GA;* [2]*Petit Institute of Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA*

ThP 528 **Detection of ions generated in an intense pulsed EUV-light beam using different interfaces to a high-resolution TOF-MS**; Niklas Pengemann[1]; Sanna Benter[1]; Maja Hammelrath[1]; Joshua Rieger[1]; Franziska Schuler[1]; Adelind Elshani[2]; Ismael Gisch[2]; Linus Nagel[2]; Hendrik Kersten[1]; Sascha Brose[2]; Carlo Holly[2]; Peter Gust[1]; Thorsten Benter[1]; [1]*University of Wuppertal, Wuppertal, Germany;* [2]*RWTH Aachen, Aachen, Germany*

ThP 529 **Lipophilic molecule analysis in a microtissue sample using supercritical fluid extraction/supercritical fluid chromatography-medium vacuum chemical ionization mass spectrometry**; Toshinobu Hondo[1, 2]; Yumi Miyake[1]; Michisato Toyoda[1]; [1]*Forefront Research Center, Graduate School of Science, Osaka University, Toyonaka, Japan;* [2]*MS-Cheminformatics, Inabe-Gun, Japan*

ThP 530 **Advancing Vacuum Matrix-Assisted Ionization (vMAI) Source for Multisample Introduction on a Portable Mass spectrometer Using 3D Printing**; Chun-Yi Lin[1]; Milan Pophristic[2]; Charles McEwen[3]; Sarah Trimpin[4]; I-Chung Lu[1]; [1]*Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan;* [2]*MSTM, LLC, Newark, DE;* [3]*University of the Sciences, Philadelphia, PA;* [4]*Wayne State University, Detroit , MI*

ThP 531 **An Autonomous, RGA Based Photoionization Mass Spectrometer for the Routine Detection of Atmospheric Trace Gasses**; Kevin A. Wokosin[1]; Steven J. Kregel[2]; Robert L. McClain[1]; Timothy H. Bertram[1]; [1]*University of Wisconsin-Madison, Madison, WI;* [2]*Bradley University, Peoria, IL*

ThP 532 **Probing ions from deeply embedded plasmas: From simulation to realization Investigation of a novel long distance ion transfer unit**; Sanna Benter[1]; Lena Mokros[1]; Markus Langner[1]; Niklas Pengemann[1]; Kersten Hendrik[1]; Thorsten Benter[1]; [1]*University of Wuppertal, Faculty of Mathematics and Natural Sciences, Wuppertal, Germany*

ThP 533 **Enhancing data quality in imaging and single-cell analysis through dopant-enriched nitrogen nebulizer gas**; Gábor Tóth[1]; Felix Friedrich[1]; Ingela Lanekoff[1]; [1]*Uppsala University, Uppsala, Sweden*

ThP 534 **Exploring a Stylus Pen as a Ion Source and Sampling Probe in Ambient Ionization Mass Spectrometry**; Yi-Ying Wu[1]; Yu-Chie Chen[1]; [1]*National Yang Ming Chiao Tung University, Hsinchu City, Taiwan*

ThP 535 **A novel multifunctional ionization source for high-efficiency native mass spectrometry**; Anthony DeBastiani[1]; Stephen Valentine[2]; Amanda DeVor[3]; Peng Li[3]; Daud Sharif[3]; Sultan Mahmud[3]; Mohammed Rahman[3]; Chong Li[3]; Kushani Attanayake[3]; [1]*WVU Department of Chemistry, Morgantown, WV;* [2]*Invibragen, Inc., Morgantown, WV;* [3]*C. Eugene Bennett Department of Chemistry; West Virginia University, Morgantown, WV*

ThP 536 **Simplified Drug Analysis: Optimizing Whole Blood Cartridge for Paper Spray Mass Spectrometry**; Greta Ren[1]; Nicholas E Manicke[1]; [1]*IUPUI, Indianapolis, IN*

ThP 537 **Separation of steroid isomers via accelerated microdroplet derivatization enabled on a custom MALDESI source**; Paul Zerebinski[1]; Xizheng Diao[2]; Ruwan T Kurulugama[3]; Sarah M Stow[3]; Richard A Yost[1]; Timothy J. Garrett[1, 4]; Boone M. Prentice[1]; [1]*University of Florida Department of Chemistry, Gainesville, FL;* [2]*University of Florida, Department of Chemistry, Gainesville, FL;* [3]*Agilent Technologies, Santa Clara, CA;* [4]*University of Florida, Department of Pathology, Immunology, and Laboratory Medicine, Gainesville, Florida*

ThP 538 **Laser Ablation Electrospray of Proteins with Ion Mobility Mass Spectrometry**; Kelcey B. Hines[1]; Neda Feizi[2]; Touradj Solouki[2]; Kermit K. Murray[1]; [1]*Louisiana State University, Baton Rouge, LA;* [2]*Baylor University, Waco, TX*

ThP 539 **Simulation of the pressure dependent Dynamic Ion Acceptance Volume (DIAV) of an electrically biased external ion sampling stage**; Markus Hübner[1]; Laura Lehmann[1]; Sanna Benter[1]; Hendrik Kersten[1]; Thorsten Benter[1]; [1]*Bergische Universität Wuppertal, Wuppertal, Germany*

ThP 540 **Kinetics of microsecond pulsed electrospray ionization**; Gavin Valdez[1]; Landon Vyhmeister[1]; Eric Davis[1]; [1]*Whitworth University, Spokane, WA*

ThP 541 **Electric Field-Modulated Electrospray Ionization Mass Spectrometry for Quantity Calibration and Mass Tracking**; Pin-Chieh Hsu[1]; Pawel L. Urban[2]; [1]*National Tsing Hua University, Hsinchu, Taiwan;* [2]*National Tsing Hua University, Hsinchu City, Taiwan*

ThP 542 **Fast, sensitive, robust, easy and quantitative direct ionization using air-permeable paper and vacuum matrix-assisted ionization (vMAI) mass spectrometry**; Hope Coffinberger[1, 2]; Charles N. McEwen[1, 2]; Sarah Trimpin[1, 3]; [1]*MSTM, LLC, Newark, DE;* [2]*Saint Joseph's University, Philadelphia, PA;* [3]*Wayne State University, Detroit , MI*

ION MOBILITY: FUNDAMENTALS
543-548

ThP 543 **Ion chemistry simulation in Traveling Wave IMS using an open simulation framework (IDSimF)**; Maja Hammelrath[1]; Michelle Rajkovic[1]; Walter Wißdorf[1]; Thorsten Benter[1]; [1]*University of Wuppertal, Wuppertal, Germany*

ThP 544 **Tailoring Separations in SLIM with Traveling Wave Gradients**; Leonard Rorrer[1]; Jim Srock[1]; Ruwan T Kurulugama[2]; Miriam Fico[1]; Daniel DeBord[1]; [1]*MOBILion Systems, Chadds Ford, PA;* [2]*Agilent Technologies, Santa Clara, CA*

ThP 545 **Effect of charge sites on biomolecule separation in ion cloud profiling method**; Zhuofan Wang[1]; Shuai Li[1]; Liwen Liang[1]; Jiexun Bu[2]; Xinwei Liu[2]; Zheng Ouyang[1]; Xiaoyu Zhou[1]; [1]*Tsinghua University, Beijing, China;* [2]*PURSPEC Technology (Beijing) Ltd., Beijing, China*

ThP 546 **Revisiting Protein Gas-Phase Unfolding: Contribution of the Mobile Proton Model through Covalent Chemical Modifications of Side Chains and Ion Mobility**; Thomas Tilmant[1]; Johann Far[1]; Edwin De Pauw[1]; Loïc Quinton[1]; [1]*ULiège, Liège, Belgium*

ThP 547 **Ion Mobility Calculations of Flexible All-Atom Systems at Arbitrary Fields Using Two-Temperature Theory**; Farah Mubas-Sirah[1]; Viraj D.Gandhi[1, 2]; Mohsen Latif[1]; Leyan Hua[1]; Amirreza Tootchi[1]; Carlos Larriba-Andaluz[1]; [1]*Indiana*

University Purdue University Indianapolis, Indianapolis, IN; [2]Purdue University, West Lafayette, IN

ThP 548 **Ion-gas collisional energy transfer between internal degrees of freedom at arbitrary fields and their effect on ion mobility**; Carlos Larriba Andaluz[1]; Viraj D Gandhi[2, 3]; *[1]IUPUI, Indianapolis, IN; [2]Indiana University Purdue University Indianapolis, Indianapolis, IN; [3]Purdue University, West Lafayette, IN*

ION MOBILITY: STRUCTURE
549-571

ThP 549 **High-resolution Ion Mobility Mass Spectrometry (HRIM MS) Empowers Diastereomer Resolution in Synthetic Phosphorothioated Oligonucleotides**; Nnenna E Dieke[1]; Joshua Shipman[1]; Cynthia Sommers[1]; Jason Rodriguez[1]; Deyi Zhang[2]; Darby Kozak[2]; Kui Yang[1]; *[1]U.S. Food and Drug Administration, Saint Louis, MO; [2]U.S. Food and Drug Administration, Silver Spring, MD*

ThP 550 **Investigating Conformational Heterogeneity of Various Caspase-9 Maturation States**; Trisha W. Brady[1]; Vanessa L. Stahl[1]; Kristalle G. Cruz[1]; Jeanne A. Hardy[1]; Richard W Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

ThP 551 **Understanding the Coordinative Selectivity of Glyphosate and AMPA Toward Divalent Metals by IM-MS and IM-IRMPD-MS**; Olivia Rusli[1]; Oscar H. Lloyd Williams[1]; Kevin Hes[2]; Sjors Bakels[2]; Anouk M. Rijs[2]; Nicole J. Rijs[1]; *[1]UNSW Sydney, Kensington, Australia; [2]Division of BioAnalytical Chemistry, Vrije Universiteit Amsterdam, Amsterdam, Netherlands*

ThP 552 **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[1]; Gordon A Anderson[2]; Alexandre A Shvartsburg[1]; *[1]Wichita State University, Wichita, KS; [2]GAA Custom Electronics LLC, Kennewick, WA*

ThP 553 **Unveiling Novel L-to-D Amino Acid Residue Isomerization in Neuropeptides via Multi-faceted Single-Cell Mass Spectrometry**; GAOYUAN LU[1]; Vu Ngoc Huong Tran[1]; Wenxin Wu[1]; Zhijun Zhu[1]; Shuling Xu[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThP 554 **Unraveling RNA Unfolding: A Comparative Study of RNA Collision Induced Unfolding and Solution-Phase Unfolding**; Anna G Anders[1]; Courteney R Dufrene[1]; Ingrid R Kilde[2]; Elizabeth E Tidwell[3]; Markos Koutmos[2, 4]; Brandon T Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, Michigan; [2]Program in Chemical Biology, University of Michigan, Ann Arbor, Michigan; [3]Program in Biophysics, University of Michigan, Ann Arbor, Michigan; [4]Program in Biophysics, University of Michigan, Ann Arbor, Afghanistan*

ThP 555 **Metal Selectivity in High-Order Complexes of Depsipeptides Investigated by a Multimodal Approach**; Thanh D Do[1]; Emmanuel Nkyaagye[2]; Miranda N. Limbach[2]; *[1]University of Tennessee, Knoxville, Knoxville, TN; [2]University of Tennessee Knoxville Chemistry Dept., Knoxville, TN*

ThP 556 **Atomic structure of an amyloidogenic segment of SOD1 with familial mutation linked to the progression of ALS**; Sarah S. Hirschbeck[1]; Michael R. Sawaya[2]; Joshua H. Jang[3]; Kristi L. Lazar Cantrell[3]; Thanh D. Do[1]; *[1]University of Tennessee, Knoxville, TN; [2]University of California, Los Angeles, Los Angeles, CA; [3]Westmont College, Santa Barbara, CA*

ThP 557 **Flow Injection-Ion Mobility-Mass Spectrometry Tracks Structural Changes in Bacterial Microcompartment Components and Reveals Mechanisms of Oligomeric Structure Assembly**; Kiani Jeacock[1]; Claudia Mak[2]; Michael R. Armbruster[1]; Anthony Vecchiarelli[2]; Brandon T. Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, Michigan; [2]Department of Molecular, Cellular, and Developmental Biology, University of Michigan, Ann Arbor, Michigan*

ThP 558 **Reduction of disulfide bonds in lysozyme monitored by ion mobility-mass spectrometry**; Sarah O'Keefe[1]; Edith Sharon[1]; Anthony J Pestritto[1]; David E. Clemmer[1]; *[1]Indiana University Bloomington, Bloomington, IN*

ThP 559 **Structural Analysis of Protein Conformational Isomers via Ion Mobility and Collision Induced Unfolding**; Michael L Moore[1]; Richard W Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

ThP 560 **Identifying the Absolute Stereochemical Configuration of Biopolymer Building Blocks with Ion Mobility-Mass Spectrometry**; Mya M Brown[1]; Ron Orlando[1]; *[1]University of Georgia, Athens, GA*

ThP 561 **Structural elucidation and capture of the early steps in α-synuclein aggregation revealed by ion mobility mass spectrometry**; Agathe Depraz Depland[1, 2]; Raya Sadighi[1, 2]; Anouk M. Rijs[1]; *[1]Vrije Universiteit Amsterdam, Division of BioAnalytical Chemistry, Amsterdam, Netherlands; [2]Centre for Analytical Sciences Amsterdam, Amsterdam, Netherlands*

ThP 562 **Peptide conformational analysis by ion mobility mass spectrometry aids drug development**; Justin Mak[1]; Pierce Jessen[1]; Amin Famili[1]; Chris M Crittenden[1]; *[1]Genentech, South San Francisco, CA*

ThP 563 **Detection of perfluoroalkyl carboxylic acid (PFCA) dimers in ion mobility spectrometry: using CCS-m/z trendlines to suggest their gas-phase conformation.**; Aurore Schneiders[1]; Johann Far[1]; Lidia Belova[2]; Edwin De Pauw[1]; Adrian Covaci[2]; Gauthier Eppe[1]; *[1]Liege University, Liège, Belgium; [2]University of Antwerp, Antwerp, Belgium*

ThP 564 **Average Charge State Analysis and Fourier Transform-Ion Mobility Provide Insights into the Conformational Dynamics of the GroEL-ATP Complex**; Kacie Evans[1]; He (Mirabel) Sun[1]; Robert L. Schrader[1]; Carter Lantz[1]; David H Russell[1]; *[1]Texas A&M University, College Station, TX*

ThP 565 **Ion mobility-based separations and selection for intact proteins enabled using native electrospray - Structures for Lossless Ion Manipulations (SLIM)**; Jung Yun Lee[1]; Yehia M. Ibrahim[1]; Stephanie M. Thibert[1]; Christopher P. Harrilal[1]; Sandilya VB Garimella[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

ThP 566 **A modified SLIM-IM-QTOF for high resolution collision induced unfolding and native protein analysis**; Ruwan T. Kurulugama[1]; Sarah M. Stow[1]; Greg Kilby[2]; Daniel DeBord[2]; Harsha Gunawardena[3]; *[1]Agilent Technologies, Santa Clara, CA; [2]MOBILion Systems, Inc., Chadds Ford, PA; [3]JOHNSON AND JOHNSON, Spring House, PA*

ThP 567 **Accurate characterization of protein structures in the gas-phase: Combining ion-mobility, molecular dynamics simulations, and enhanced energy landscape sampling methods**; Viraj D Gandhi[1, 2]; Morgan Lawrenz[3]; Iain D.G. Campuzano[4]; Carlos Larriba-Andaluz[1]; *[1]Indiana University Purdue University Indianapolis, Indianapolis, IN; [2]Purdue University, West Lafayette, IN; [3]Schrödinger, Inc, San Diego, CA; [4]Amgen, Thousand Oaks, CA*

ThP 568 **Assembly and disassembly of multimeric states in the QueD2 system**; Colin R Johnson[1]; Emma M. McRae[1]; Matthew R. Jordan[1]; Giovanni Gonzalez-Gutierrez[1]; Jonathan C. Trinidad[1]; David P. Giedroc[1]; David E. Clemmer[1]; *[1]Indiana University, Bloomington, IN*

ThP 569 **Structural Identification of Small Molecules, Peptides, Proteins, and Complexes via nESI-TIMS-q-UVPD-FTICR MS/MS**; Samuel A Miller[1]; Kevin Jeanne Dit Fouque[1]; Miguel Santos[1]; Mark E Ridgeway[2]; Steve Van Orden[3]; Francisco A Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]Bruker Scientific, LLC, Billerica, MA; [3]Bruker Daltonics Inc., Billerica, MA*

ThP 570 **Ion mobility reveals intriguing solvent effects on lossless Intramolecular proton transfers in gaseous ion ensembles**; Athula B. Attygalle[1]; Meenu Kumar[1]; *[1]Stevens Institute of Technology, Hoboken, NJ*

ThP 571 **All Multispecific-Antibodies Undergo Large and Measurable Levels of Gas-Phase Collapse**; Iain D G

Campuzano[1]; CHEN-CHUN CHEN[2]; *[1]Amgen Inc., Thousand Oaks, CA; [2]Eli Lilly and Company, Indianapolis, IN*

LC/MS: GENERAL
572-600

ThP 572 **Optimization of LC-MS Method Development for Efficient Quantification of CYP Metabolites: A QTOF based Mass Spectrometry Approach**; Zarna A Raichura[1]; Kabre Heck[1]; Angela Calderon[1]; *[1]Auburn University, Auburn, AL*

ThP 573 **Influence of gas impurities on electrospray spectra background noise**; Tomasz Bienkowski[1, 2]; Konrad Kowalski[2, 3]; *[1]LNI SWISSGAS EE sp. z o.o., Warszawa, Poland; [2]Masdiag Sp. z o.o., Warsaw, Poland; [3]MS Ekspert Sp. z o.o., Gdańsk, Poland*

ThP 574 **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[1]; Kumari Ubhayasekera[1]; Jonas Bergquist[1]; *[1]Uppsala University, Uppsala, Sweden*

ThP 575 **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[1]; Husam Kafeenah[1]; Quynh-Trang Do[1]; Fung-Yu Chen[1]; *[1]National Cheng Kung University, Tainan, Taiwan*

ThP 576 **Method Development of Sample Preparation and HPLC Separation for the Characterization of Peptide-RNA Conjugates via LC-MS**; Christopher Kovach[1]; Guihong Qi[1]; Xianyin Lai[1]; *[1]Eli Lilly & Company, Indianapolis, IN*

ThP 577 **Quality Control of Newly Synthesized Small Molecules and Peptides Using High Throughput UPLC-MS**; Wilfredo Pinto[1]; Foster Tenkorang[1]; *[1]Merck, Rahway, NJ*

ThP 578 **Agilent RoHS Compliant Ion Injector for LCMS Single Quadrupole and Triple Quadrupole Instruments**; Samuel Haddad[1]; Jennifer Sanderson[2]; Paul Tripp[3]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies Inc., Santa Clara, CA; [3]Agilent Technologies, Santa Clara, CA*

ThP 579 **Dipolarity Polarity Component of the Mobile Phase: A Crucial Factor in the Separation of Bile Acid Enantiomers in RPLC-MS**; Mst Ummul Khair[1]; David Anderson[2]; *[1]cleveland state university, Cleveland, OH; [2]Cleveland State university, CLEVELAND, OH*

ThP 580 **Lipid Characterization of Extracellular Vesicles Released by Drug-resistant Leishmania Parasites**; Erica Kim[1]; Ana Victoria Ibarra-Meneses[2]; Alisa Hui[1]; Christopher Fernandez Prada[2]; Tao Huan[1]; *[1]University of British Columbia, Vancouver, BC; [2]University of Montreal, Montreal, QC*

ThP 581 **Troubleshooting and Counteracting Quetiapine-Induced Interference in LC-MS/MS analysis**; Jongsun Joo[1]; Ju Hyeong Lee[1]; Jikyo Lee[1]; Sang Hoon Song[1]; *[1]Seoul National University Hospital, Seoul, South Korea*

ThP 582 **An Alternative Approach for NDMA Quantification in Metformin Final Product by LC/MS Single Quadrupole**; Lucas Lima Zanin[1]; Marcos Albieri Pudenzi[1]; Ichiro Hirano[2]; *[1]Shimadzu do Brasil, Barueri, Brazil; [2]Shimadzu do Brasil, Barueri, Brazil*

ThP 583 **Enabling faster MRM while maintaining instrument robustness**; David Cox[1]; Yang Kang[1]; Ian Moore[1]; Holly Lee[1]; Michael Deng[1]; *[1]SCIEX, Concord, ON*

ThP 584 **Pushing the flexibility of Multi-task analysis: The challenges of an MS facility are wide-ranging projects on limited instrumentation**; Reynard A Spiess[1]; Katherine Hollywood[1]; Aliaksandr Baidak[1]; Jaleel Miyan[1]; Harmesh Aojula[1]; Shaymaa Mudhaffer[1]; Elen Clayton[1]; Vishal Kawale[1]; *[1]University of Manchester, Manchester, United Kingdom*

ThP 585 **A 3D-printed serpentine column for size exclusion chromatography separations with mass spectrometric detection**; Olanrewaju Awoyemi[1]; Jing Wang[1]; Madison Pursell[1]; Amanda DeVor[1]; Riley White[1]; Stephen J Valentine[1]; Peng Li[1]; *[1]West Virginia University, Morgantown, WV*

ThP 586 **Development of a Desalination Tube for an On-line LC/MS Analysis**; Yutaka Takahashi[1, 2, 3]; Sachiki Shimizu[3]; Takumi Sakamoto[1]; Mitsutoshi Setou[1, 2]; *[1]Hamamatsu University School of Medicine, Shizuoka, Japan; [2]Preppers Co. Ltd, Shizuoka, Japan; [3]MS-Solutions Co. Ltd., Tokyo, Japan*

ThP 587 **High-Throughput Quantification of Vitamin D Metabolites in Dried Blood Spots**; Keeley Jo Alexander[1]; Kavinda DeSilva[1]; Frances Morris[1]; Zane Hauck PhD[1]; *[1]Molecular Testing Labs, Vancouver, WA*

ThP 588 **Lifetime Testing of Novel RoHS Compliant Ion Injectors with Real-time Early Maintenance Feedback (EMF) Diagnostic Monitoring on Multiple LC/TQ Platforms**; Sampada Borkar[1]; Michael B Pastor[1]; Ryan Rademacher[1]; Paul Tripp[1]; *[1]Agilent Technologies, Santa Clara, CA*

ThP 589 **Antisense oligonucleotide extraction optimization reveals significant differences between non-human primate spinal cord, mouse spinal cord, and mouse brain tissue homogenates**; Brandon M Davies[1]; Brandon Wilcock[1]; Terry Fang[2]; Brian Bettencourt[2]; Troy Voelker[1]; *[1]Aliri Bioanalysis, Salt Lake City, UT; [2]Third Rock NewCo, Boston, USA, MA*

ThP 590 **New HESI sprayer design for improved precision and robustness across all source temperature/gas ranges**; Charles Maxey[1]; Cornelia Boeser[1]; Neloni Wijeratne[1]; Eloy R. Wouters[1]; Brian Adamson[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 591 **Evaluating Diverse Modalities for LC-MS/MS Quantitation Across Three Sciex Triple Quadrupole Platforms**; Carla Camou-Sainz[1]; Darian Bartkowski[1]; Alyssa Gillies[1]; *[1]Takeda, San Diego, CA*

ThP 592 **Open-tubular trap columns: towards simple and robust liquid chromatography separations for single-cell proteomics**; Siqi Huang[1]; Kei Webber[1]; Thy Truong[1, 2]; Jacob Heninger[1]; Ryan T. Kelly[1, 2]; *[1]Brigham Young University, Provo, UT; [2]MicrOmics Technologies, Spanish Fork, UT*

ThP 593 **Trace level estimation of N-Nitroso Isavuconazonium Sulphate in Isavuconazonium Sulphate API using liquid chromatography and nominal mass tandem mass spectrometry**; Ian Edwards[1]; Saikat Bhattacharya[2]; Prasanth Joseph[2]; Vivek Dhyani[3]; Saikat Banerjee[4]; *[1]Agilent Technologies Inc., Santa Clara, CA; [2]Agilent technologies, Bangalore, India; [3]Agilent Technologies, Mumbai, India; [4]Agilent Technologies, Hyderabad, India*

ThP 594 **Sensitive and selective quantitation of N-nitroso dabigatran etexilate impurity (NDSRI) in dabigatran drug substance at picogram levels using LC/MS/MS**; Parul Angrish[1]; Preeti Bharatiya[2]; Prasanth Joseph[2]; Vivek Dhyani[3]; Saikat Banerjee[4]; Kannan Balakrishnan[2]; *[1]Agilent Technologies Inc., Santa Clara, USA; [2]Agilent Technologies Inc., Bangalore, India; [3]Agilent Technologies Inc., Mumbai, India; [4]Agilent Technologies Inc., Hyderabad, India*

ThP 595 **Utilization of the speed, sensitivity and accuracy of the ZenoTOF 7600 to enhance protein identifications from packed emitter columns**; Sri Ramarathinam[1]; Aaron Poth[2]; Mohammadreza Dorvash[1]; Patricia Illing[1]; Jarrod Sandow[2]; Anthony Purcell[1]; *[1]Monash University, Clayton, Australia; [2]IonOpticks, Fitzroy, Australia*

ThP 596 **Determination of Paraquat in Drinking Water by LCMS-2050**; Marilia Santoro Cardoso[1]; Marcos A Pudenzi[2]; Luisa B Ambrosio[2]; Ichiro Hirano[2]; *[1]Shimadzu do Brasil, Barueri - SP, Brazil; [2]Shimadzu do Brasil, Barueri, Brazil*

ThP 597 **Simultaneous quantitation of N-nitrosamines and NDSRIs in formulation samples by using a DUIS ionization source in LC-MS/MS**; Nitish Ramchandra Suryawanshi[1]; Samruddha Chavan[1]; Nitin Shukla[1]; Devika Tupe[1]; Siddhesh Ghadi[1]; Shalu Nair[1]; Jitendra Kelkar[1]; Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

ThP 598 **Quantification of potentially toxic chemicals in simulated leachate from four widely used tire-derived materials by LC/MS/MS**; Jonathan Navarro Ramos[1]; John

D. Atkinson[2]; Joshua Wallace[1]; Diana S Aga[1]; James Lang[2]; Phillip Zimako Onyeme[2]; [1]*Department of Chemistry, The State University of New York at Buffalo, Buffalo, NY;* [2]*Department of Civil, Structural, and Environmental Engineering, The State University of New York at Buffalo, Buffalo, NY*

ThP 599 **Stability indicating LC-MS/MS method for estimation of Bromocriptine mesylate in human plasma application to a bioequivalence study**; Narendra Kumar Reddy Kolli[1]; Swetha Polagani[1]; Arya Lakshmi Marisetti[2]; [1]*Sri Vani School Of Pharmacy, Vijayawada, India;* [2]*Delhi Pharmaceutical Sciences and Research University, New Delhi, India*

ThP 600 **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[1]; Narendra Kumar Reddy Kolli[2]; Murali Krishna Kumar Muthyala[3]; [1]*Sri Vani School Of Pharmacy, Vijayawada., India;* [2]*Sri Vani School Of Pharmacy, Vijayawada, India;* [3]*Andhra University College Of Pharmaceutical Sciences, Visakhapatnam, India*

LIPIDS: TARGETED AND QUANTITATIVE ANALYSIS
601-633

ThP 601 **The Innovation Solution of Eicosanoids and Related Oxylipins Profiles as Biomarkers by LC-MS/MS in Uterine Fibroids Disease**; Ting-Li Han[1]; Xin Wang[1]; Xiao-Rong Ran[2]; Yue Song[3]; Shan-An Chan[4]; [1]*State Key Laboratory of Ultrasound in Medicine and Engineering, College of Biomedical Engineering, Chongqing Medical University, Chongqing, China;* [2]*Agilent Technologies Inc., Beijing, China;* [3]*Agilent Technologies Inc., Shanghai, China;* [4]*Agilent Technologies Inc., Taipei, China*

ThP 602 **Estimation of positional lipid isomers in a biological mixture using Parallel Reaction Monitoring (prm) and isomer quantification model**; Dhanwin Baker[1]; Laura Bindila[1]; [1]*University Medical Center of Mainz, Mainz, Germany*

ThP 603 **Application of Targeted Lipidomics to Determine Changes in the Plasma Lipidome of Male Rats Follow Repeat Oral Administration of Methapyrilene**; Robert Plumb[1]; Ian D Wilson[2]; Andrew Leightner[3]; Anthony J Midey[3]; Steven K Lai[3]; Roy Martin[4]; [1]*Waters, Milford, MA;* [2]*Imperial College London, London, United Kingdom;* [3]*Waters Corporation, Milford, MA;* [4]*Waters Corporation, Milford, Massachusetts*

ThP 604 **Intramolecular Paternò-Büchi reaction coupled with isobaric tagging for parallel quantitation of fatty acids at multiple structural levels**; Lipeng Qiao[1]; Hengxue Shi[1]; Yichun Wang[1]; Yu Xia[1]; [1]*Tsinghua University, Beijing, China*

ThP 605 **LICAR2: automated isotopic correction tool for targeted lipidomic data acquired with class-based chromatographic separations using multiple reaction monitoring**; Liang Gao[1]; Shanshan Ji[1]; Amaury Cazenave-Gassiot[1]; Bo Burla[1]; [1]*National University of Singapore, Singapore, Singapore*

ThP 606 **Targeted lipidomics of a randomized crossover trial with human subjects**; Nara Marella[1]; Matthäus Metz[2]; Marianna Beghini[2]; Peter Wolf[2]; Lorenz Pfleger[2]; Martina Hackl[2]; Magdalena Bastian[2]; Angelika Freudenthaler[2]; Juergen Harreiter[2]; Maximilian Zeyda[3]; Sabina Baumgartner-Parzer[2]; Rodrig Marculescu[4]; Thomas Hannich[5]; Georg Gyoeri[6]; Gabriela Berlakovich[6]; Michael Roden[7]; Micahel Krebs[2]; Robert Risti[8]; Aivar Lõokene[9]; Michael Trauner[10]; Alexandra Kautzky-Willer[2]; Martin Krššák[2]; Herbert Stangl[11]; Clemens Fürnsinn[2]; Thomas Scherer[2]; [1]*CeMM Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria;* [2]*Division of Endocrinology and Metabolism, Department of Internal Medicine III, Medical University of Vienna, Vienna, Austria;* [3]*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;* [4]*Department of Laboratory Medicine, Medical University of Vienna, Vienna 1090, Austria, Vienna, Austria;* [5]*CeMM Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria;* [6]*Division of Transplantation, Department of Surgery, Medical University of Vienna, Vienna 1090, Austria, Vienna, Austria;* [7]*Division of Endocrinology and Diabetology, Medical Faculty and University Hospital, Heinrich Heine University, Düsseldorf 40225, Germany, Duessldorf, Germany;* [8]*Department of Chemistry, Tallinn University of Technology, Tallinn 12618, Estonia, Estonia, Estonia;* [9]*Department of Chemistry, Tallinn University of Technology, Tallinn 12618, Estonia, Estonia, Austria;* [10]*Division of Gastroenterology and Hepatology, Department of Internal Medicine III, Medical University of Vienna, Vienna 1090, Austria, Vienna, Austria;* [11]*Institute of Medical Chemistry, Center for Pathobiochemistry and Genetics, Medical University of Vienna, Vienna 1090, Austria, Vienna, Austria*

ThP 607 **Investigation of PLA2 Inhibitors' Influence on Enzymatic and Non-Enzymatic Oxidized Phospholipids in Immortalized Microglial Cells**; Sazia Arefin Kachi[1]; Yulemni Morel[1]; Amir Mehrabani Tabari[2]; Nivedita Hegdekar[2]; Chinmoy Sarkar[2]; Marta M. Lipinski[2]; Jace W. Jones[1]; [1]*University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD;* [2]*University of Maryland, School of Medicine, Department of Anesthesiology, Baltimore, MD*

ThP 608 **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[1]; Yulia Y Tyurina[1]; Rina Kim[2]; Ayumi Hashimoto[3]; Valerian E Kagan[4]; Dmitry I Gabrilovich[3]; Yulia Nefedova[5]; [1]*University of Pittsburgh, Pittsburgh, PA;* [2]*University of Pennsylvania, Philadelphia, PA;* [3]*AstraZeneca, Gaithersburg, MD;* [4]*University of Pittsburgh, Pittsburgh, Pennsylvania;* [5]*Wistar Institute, Philadelphia, PA*

ThP 609 **The lipoprotein-associated phospholipase A2 inhibitor Darapladib sensitises cancer cells to ferroptosis by remodelling lipid metabolism**; Seoyoung Jang[1]; Mihee Oh[2]; Ji-Yoon Lee[2]; Eun-Woo Lee[2]; Geum-Sook Hwang[1]; [1]*Korea Basic Science Institute, Seoul, South Korea;* [2]*Korea Research Institute of Bioscience and Biotechnology, Daejeon, South Korea*

ThP 610 **Investigate Skin Fibroblasts Lipidome Changes in Optic Disc Drusen Using a Comprehensive Targeted LC-dMRM Method**; Mengying Fu[1]; Yuqin Dai[1]; Karanvir Kaushal[2]; Yaping Joyce Liao[2]; [1]*Sarafan ChEM-H, Stanford University, Stanford, CA;* [2]*Department of Ophthalmology, Stanford University, Stanford, CA*

ThP 611 **A high efficiency quantitation method for aldehyde-containing compounds based on chemical isotope-coded derivatization**; XIAOHUI FENG[1]; Zhenghua Rao[1]; Yaxiong Jia[1]; [1]*Institute of Animal Sciences, CAAS, Beijing, China*

ThP 612 **Elevated levels of arachidonic acid containing lipids underlie cardiovascular disease risk in White and Black Females**; Raghav Jain[1]; Jessica W Davidson[1]; Dominique A Baldwin[1]; Judith Simcox[1]; [1]*University of Wisconsin-Madison, Department of Biochemistry, Madison, WI*

ThP 613 **Comprehensive shotgun lipidomics workflow using SLA platform and LipStR for the lipid profiling of human milk**; Weng Wong[1]; James Joubert[1]; Meena Choi[1]; William Dishen Liu[1]; Anatoly Belov[1]; Jay Leone[1]; Wendy Sandoval[1]; Qingling Li[1]; [1]*Genentech, South San Francisco, CA*

ThP 614 **Unleashing High Sensitivity: NanoLC Monolithic Columns in 4D Metabolomics and Lipidomics**; Tina McGuire[1]; Michael Krawitzky[2, 3]; Erica Marie Forsberg[1]; Goran Mitulovic[3]; Matthew R Lewis[4]; [1]*Bruker Scientific, LLC, Billerica, MA;* [2]*Bruker Daltonics, San Jose, CA;* [3]*Bruker Switzerland AG, Faellanden, Switzerland;* [4]*Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany*

ThP 615 **Optimization of a sensitive method for quantifying dicarboxylic acids using liquid chromatography tandem mass spectrometry**; Joby Jose[1]; Alfred N Fonteh[1]; [1]*Huntington Medical Research Institutes, Pasadena, CA*

ThP 616 **High-Throughput Mass Spectrometry Assay Platform for Characterizing Selectivity of Small Molecule Inhibitors Against Multiple Enzymes in the Cholesterol Biosynthesis Pathway**; Ronghai Cheng[1]; Reza Nemati Josheghani[1]; Daniel Tekverk[1]; Howard Jones[1]; Martin Himmelbauer[1]; *[1]Biogen, Cambridge, MA*

ThP 617 **Profiling of glycosphingolipids and gangliosides from dried bloodspots for diagnosis of inherited genetic disorders**; Jinyong Kim[1]; Seul Kee Byeon[1]; Akhilesh Pandey[1]; *[1]Mayo Clinic, Rochester, MN*

ThP 618 **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[1]; Katarzyna Dorota Wrobel[1]; Oracio Serrano Torres[1]; Kazimierz Wrobel[1]; *[1]University of Guanajuato, Guanajuato, Mexico*

ThP 619 **Base Hydrolysis (or Not) for Targeted Sphingolipid Quantitation**; Josie Daldegan Rezende[1]; Yuanyuan Ji[1]; Anh Tran[1]; Jace W. Jones[1]; *[1]University of Maryland, Baltimore, Baltimore, MD*

ThP 620 **Identifying Dysregulated Lipids in Human Brain of Alzheimer's Disease and their Effects on Biological Pathways**; Akeem Sanni[1]; Andrew I Bennett[1]; Moyinoluwa Adeniyi[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

ThP 621 **Ferroloxins inhibit phosphatidylethanolamine oxidation catalyzed by 15LOX/PEBP1 complex in vitro and in vivo and mitigate ferroptosis**; Yulia Y. Tyurina[1]; Haider H. Dar[1]; Karolina Mikulska-Ruminska[2]; Diane K. Luci[3]; Adam Yasgar[3]; Svetlana N. Samovich[4]; Kapralov A Alexander[1]; Austin B. Souryavong[1]; Vladimir A. Tyurin[1]; Andrew A Amoscato[1]; Louis J. Sparvero[1]; Ecem Saritas[1]; Mert Akdogan[1]; Michael W Epperly[1]; Galina V. Shurin[1]; Melissa Standley[5]; Theodore R Holman[5]; Claudette M. St. Croix[1]; Simon C. Watkins[1]; Andrew P. VanDemark[1]; Sandeep Rana[3]; Alexey V. Zakharov[3]; Anton M. Simeonov[3]; Rama K. Mallampalli[6]; Sally E. Wenzel[1]; Joel S. Greenberger[1]; Ganesha Rai[3]; Hülya Bayir[4]; Ivet Bahar[7]; Valerian E Kagan[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Nicolaus Copernicus University, Bydgoszcz, Poland; [3]National Center for Advancing Translational Sciences (NCATS), Rockville, MD; [4]Columbia University Irving Medical Center, New York, NY; [5]University of California Santa Cruz, Santa Cruz, CA; [6]The Ohio State University, Columbus, OH; [7]Stony Brook University, Stony Brook, NY*

ThP 622 **Impact of chronic exposure to environmentally relevant micro/nanoplastics on mouse lipidome by D2O metabolic labeling**; Jonghyun Kim[1]; Jinyoung Park[1]; Hyoun Hyoung Jang[1]; Sokkhornn Phorn[1]; Tae-Young Kim[1]; *[1]School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea*

ThP 623 **Targeted method of polyprenols and dolichols using ion trap-based higher energy collision-induced dissociation**; Seul Kee Byeon[1]; Jinyong Kim[1]; Rahul R Deshpande[2]; Susan S. Bird[2]; Akhilesh Pandey[1]; *[1]Mayo Clinic, Rochester, MN; [2]ThermoFisher Scientific, San Jose, CA*

ThP 624 **Breaking Limits: Nanoscale LC-TIMS-MS Empowers Low Sample Volume Single-Cell 4D-Lipidomics**; Rebekah J Woolsey[1]; Michael Krawitzky[2, 3]; Irina Maerki[3]; Florian Busch[3]; Sven W Meyer[4]; Erica Marie Forsberg[5]; Claudia Martinelli[3]; Jean-François Greisch[3]; Matthew R Lewis[4]; *[1]University of Nevada Reno, Reno, NV; [2]Bruker Daltonics, San Jose, CA; [3]Bruker Switzerland AG, Faellanden, Switzerland; [4]Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, 28359 Bremen, Germany; [5]Bruker Scientific, LLC, Billerica, MA*

ThP 625 **Fatty acids positional isomers quantification using nanospray Supercritical Fluid Chromatography-Mass Spectrometry (nSFC-MS)**; Mahmoud Elhusseiny Abdelrahman Mostafa[1]; John R Boughton[2]; James P Grinias[2]; James Edwards[1]; *[1]Saint Louis University, Saint Louis, MO; [2]Rowan University, Glassboro, New Jersey*

ThP 626 **Comprehensive Analysis of Signaling Lipids in Biological Matrices Using Metal-free LC-MS/MS**; Stefanie Rubenzucker[1, 2]; Mailin-Christin Manke[3, 4]; Rainer Lehmann[5]; Alice Assinger[6]; Oliver Borst[3, 4]; Robert Ahrends[1]; *[1]Department of Analytical Chemistry, University of Vienna, Vienna, Austria; [2]Vienna Doctoral School in Chemistry (DoSChem), University of Vienna, Vienna, Austria; [3]Department of Cardiology and Angiology, University of Tuebingen, Tuebingen, Germany; [4]DFG Heisenberg Group Cardiovascular Thromboinflammation and Translational Thrombocardiology, University of Tuebingen, Tuebingen, Germany; [5]Institute for Clinical Chemistry and Pathobiochemistry, Department for Diagnostic Laboratory Medicine, University Hospital Tuebingen, Tuebingen, Germany; [6]Department of Vascular Biology and Thrombosis Research, Centre of Physiology and Pharmacology, Medical University of Vienna, Vienna, Austria*

ThP 627 **High-throughput, quantitative targeted lipidomic method for large-scale measurement of lipids in human plasma samples**; Yuanyuan Ji[1]; Yulemni Morel[1]; Anh Tran[1]; Jace W. Jones[1]; *[1]University of Maryland, Baltimore, Baltimore, MD*

ThP 628 **Towards targeted and quantitative 4D Lipidomics - From PASEF to prm-PASEF**; Edward Rudt[1]; Viola Jeck[2]; Nikolas Kessler[2]; Christian Müller[2]; Ilmari Krebs[2]; Heiko Neuweger[2]; Heiko Hayen[1]; *[1]University of Muenster, Institute of Inorganic and Analytical Chemistry, Münster, Germany; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

ThP 629 **The lysophosphatidylcholine is an essential and versatile source for de novo phospholipids' biosynthesis in Plasmodium falciparum**; Corinne BURE[1]; Quentin Chevalier[2]; Sharon Wein[2]; Rachel Cerdan[2]; *[1]CNRS - IECB, Pessac, France; [2]Montpellier University, MONTPELLIER, France*

ThP 630 **Wide-scope targeted analysis of bioactive lipids by LC/MS/MS**; Kohta Nakatani[1]; Yoshihiro Izumi[1]; Hironobu Umakoshi[2]; Maki Yokomoto-Umakoshi[2]; Tomoko Nakaji[1]; Hiroki Kaneko[2]; Hiroshi Nakao[2]; Yoshihiro Ogawa[2]; Kazutaka Ikeda[3]; Takeshi Bamba[1]; *[1]Medical Institute of Bioregulation, Kyushu University, 3-1-1 Maidashi, Higashi-ku, Fukuoka-shi, Japan; [2]Department of Medicine and Bioregulatory Science, Graduate School of Medical Sciences, Kyushu University, Fukuoka, Japan; [3]Kazusa DNA Research Institute, 2-6-7 Kazusakamatari, Kisarazu, Japan*

ThP 631 **The New Normal: Evidence for why we should stop using protein concentration for lipid normalization in quantitative lipidomics**; Kari B Basso[1]; Laura Bailey[2]; *[1]University of Florida, Gainesville, FL; [2]University of Florida, Department of Chemistry, Gainesville, FL*

ThP 632 **LC-MRM-MS profiling of oxylipins and fatty acids in human milk after hydrolysis**; Liping Yang[1]; Jaewoo Choi[1]; David C. Dallas[2]; Jan F. Stevens[3, 4]; Claudia S. Maier[1, 4]; *[1]Department of Chemistry, Oregon State University, Corvallis, OR; [2]Nutrition Program, College of Health, Oregon State University, Corvallis, OR; [3]Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR; [4]Linus Pauling Institute, Oregon State University, Corvallis, OR*

ThP 633 **LC-MS/MS analysis of glucosylceramides (GlcCer) and glucosylsphingosine (GlcSph) in L444P fibroblast cells**; Nicole E Bebrin[1]; Sho Sato[1]; Shin-ichi Matsumoto[2]; Hiroshi Sugimoto[1]; *[1]Takeda Pharmaceuticals, Cambridge, MA; [2]Takeda Pharmaceutical Company Limited, Fujisawa, Japan*

MALDI: APPLICATIONS
634-644

ThP 634 **Determining the stability of botulism clinical specimens using MALDI-TOF mass spectrometry**; Victoria Foltz[1]; Kiara Gonzalez-Colon[1, 2]; Janet Dykes[1]; Andre Hopkins[1]; Carolina Luquez[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA; [2]ASRT, Inc, Atlanta, GA*

ThP 635 **Analysis of Heavy Metals Using Porphyrin Decorated Hydrophobic Materials Coupled with MALDI-MS Measurement**; Hsin-You Tseng[1]; He-Hsuan Hsiao[1];

[1]*Department of Chemistry, National Chung Hsing University, Taichung, Taiwan*

ThP 636 **C18-functionalized Manganese Ferrite Magnetic Nanoparticles in Combination with LDI-MS for the Analysis of Malachite Green**; Chang-En Lee[1]; He-Hsuan Hsiao[1]; [1]*Department of Chemistry, National Chung Hsing University, Taichung, Taiwan*

ThP 637 **An Optimized MALDI Assay for Tree Gum Discrimination in Works of Art**; Katherine J Kenney[1]; Daniel D. Vallejo[1]; Katell Bathany[2, 3]; Caroline Tokarski[2, 3]; Facundo M. Fernandez[1]; [1]*Georgia Institute of Technology, Atlanta, GA;* [2]*University of Bordeaux, CNRS, Bordeaux INP, CBMN, UMR 5248, Pessac, France;* [3]*Bordeaux Proteome Platform, University of Bordeaux, Bordeaux, France*

ThP 638 **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[1]; Linda Vu[1]; Moira Overly[1]; Hyojik Yang[1]; Richard D. Smith[1]; Matthew E. Sherman[1]; DAVID R GOODLETT[2]; Charles R. Sweet[3]; ROBERT K ERNST[1]; [1]*University of Maryland, Baltimore, Baltimore, MD;* [2]*University of Victoria, Victoria, BC;* [3]*United States Naval Academy, Annapolis, MD*

ThP 639 **MALDI imaging of Drosera capensis indicates changes in abundance and spatial distribution of biomolecules after induced digestion**; Jonathan V. Le[1]; Zane G. Long[1]; Rachel W. Martin[1]; [1]*University of California, Irvine, Irvine, CA*

ThP 640 **Interfacial Dynamics: Molecular Insights into Cacao Butter Phospholipids and their Influence on Water/Oil Emulsion Stability**; Luis M. Díaz-Sánchez[1]; Laura A. Paiba[1]; Luis G. Gómez-Martínez[2]; Aldo F. Combariza[2]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza[1]; [1]*Universidad Industrial de Santander, Bucaramanga, Colombia;* [2]*Universidad de Sucre, Sincelejo, Colombia*

ThP 641 **Evaluating association of perfluorooctanesulfonic acid (PFOS) to bacteria using MALDI-MS**; Irfath Jasmin Reza[1]; Tian Autumn Qiu[1, 2]; [1]*Michigan State University Department of Chemistry, East Lansing, MI;* [2]*MSU Center for PFAS Research, East Lansing, Michigan*

ThP 642 **Unraveling Phytoplankton Communities in a Marine Ecosystem through MALDI-FT-ICR Profiling**; Luis M. Díaz-Sánchez[1]; Martha L. Chacón-Patiño[2]; Chad R Weisbrod[2]; Julián Franco[3]; Lizbeth J. Vivas-Aguas[3]; David Stranz[4]; Scott Campbell[4]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza[1]; [1]*Universidad Industrial de Santander, Bucaramanga, Colombia;* [2]*National High Magnetic Field Laboratory, Tallahassee, FL;* [3]*Marine and Coastal Research Institute-INVEMAR, Santa Marta, Colombia;* [4]*Sierra Analytics, Modesto, California*

ThP 643 **AP/MALDI with high resolution and triple quadrupole mass analyzers for sensitive and high-throughput food authenticity analysis**; Nivedita Bhattacharya[1, 2]; Vishal Mahale[1, 2]; Madhuri Gupta[1, 2]; Nasiruddin Sheikh[3]; Akshay Vasekar[3]; Madhura Thete[2]; Enrico Davoli[4]; Kaushik Banerjee[3]; Venkateswarlu Panchagnula[1, 2]; [1]*MassTech Inc., Columbia, MD;* [2]*Barefeet Analytics Pvt. Ltd., Pune, India;* [3]*ICAR-National Research Centre for Grapes, Manjiri Farm, P B, No 3, Solapur Rd, Pune, Maharashtra 412307, India, Pune, India;* [4]*Mario Negri Institute for Pharmacological Research, Via Mario Negri, 2, 20156 Milano MI, Italy, Europe, Milano, Italy*

ThP 644 **Advances in block copolymer materials research enabled by MALDI-TOF mass spectrometry**; Alyssa W May[1]; Joseph G Luther[1]; Travis S Bailey[1]; [1]*Colorado State University, Fort Collins, CO*

MALDI: INNOVATION IN INSTRUMENTATION AND SAMPLE PREPARATION
645-650

ThP 645 **Burst Nucleation of Matrix on Doped Graphene for Quantitative MALDI-ToF Mass Spectrometry with Tunable Ion Yield**; Sanghwan Park[1]; Chang Young Lee[1]; [1]*Ulsan National Institute of Science and Technology, Ulsan, South Korea*

ThP 646 **A Plug-and-Play Laser Post-Ionization Module for AP-MALDI-2 Orbitrap Mass Spectrometry Imaging with Improved Sensitivity**; Maureen Feucherolles[1]; Olivier Bouton[2]; Mathieu Gérard[2]; Eugene Moskovets[3]; Gilles Frache[1]; [1]*Luxembourg Institute of Science and Technology, Molecular and Thermal Analysis, Belvaux, Luxembourg;* [2]*Luxembourg Institute of Science and Technology, Conception & prototyping, Belvaux, Luxembourg;* [3]*MassTech Inc., Columbia, MD*

ThP 647 **Centrifuge Tube Filters for Effective Bacterial Capture and Lysis from Biofluids for MALDI-based Mass Fingerprinting**; Austin R. Anderson[1]; Erick S. LeBrun[1]; Nileena Velappan[1]; Emilio S. Rivera[1]; Kes A. Luchini[1]; Ethan M McBride[2]; Trevor G. Glaros[1]; [1]*Biochemistry and Biotechnology Group, Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM;* [2]*Los Alamos National Laboratory, Los Alamos, NM*

ThP 648 **Analysis of Small Biomolecules Aided by a Broad-Spectrum Reactive/Electron-Transfer Matrix; Covalent Radical Generating (CovRAGE) MALDI**; Cameron J Kaminsky[1]; Hua Zhang[2]; Lingjun Li[1, 2]; [1]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [2]*School of Pharmacy, Madison, Wisconsin*

ThP 649 **Sample preparation method for fresh-frozen, undecalcified rat spine for MALDI MSI**; Kayle J Bender[1]; Yongheng Wang[2]; Chuo Ying Zhai[1]; Zoe Saenz[3]; Aijun Wang[4, 5]; Elizabeth K Neumann[1]; [1]*Department of Chemistry, University of California, Davis, Davis, California;* [2]*Department of Biomedical Engineering, University of California, Davis, California;* [3]*Department of Surgery, School of Medicine, University of California, Davis, Sacramento, California;* [4]*Center for Surgical Bioengineering, Department of Surgery, School of Medicine, University of California, Davis, Sacramento, California;* [5]*nstitute for Pediatric Regenerative Medicine, Shriners Hospital for Children Northern California, UC Davis School of Medicine, Sacramento, California*

ThP 650 **Exchange of Buffer System for MALDI-MS Analysis of Oligonucleotides without Desalting**; Andreas Baumeister[1]; Ido Bachelet[2]; Ronen Weiss[2]; [1]*Shimadzu Europa GmbH, Duisburg, Germany;* [2]*Augmanity Nano Ltd, Rehovot, Israel*

METABOLOMICS: TARGETED AND QUANTITATIVE ANALYSIS II
651-672

ThP 651 **Effects of Dietary Docosahexaenoic Acid on Lipid Peroxidation Products in Mice Brain**; Kate Nyarko[1]; Michael Greenlief[1]; [1]*University of Missouri-Columbia, Columbia, MO*

ThP 652 **Establishing an energy-related metabolism platform using cyanopropyl-based LC-MS/MS**; Wan-Rou Liao[1]; Sung-Fang Chen[2]; [1]*National Taiwan Normal Universit, Taipei, Taiwan;* [2]*National Taiwan Normal University, Taipei, Taiwan*

ThP 653 **Quantification of Cyanogenic Glycosides using LC-MS/MS MRM**; Zhentian Lei[1]; Deepak Kasote[1]; Clayton D. Kranawetter[1]; Ashley C. Conway-Anderson[1]; Barbara W. Sumner[1]; Lloyd W. Sumner[1]; [1]*University of Missouri, Columbia, MO*

ThP 654 **Quantitative and qualitative analysis of steroids by high-resolution mass spectrometry**; Robert Proos[1]; Paul RS Baker[1]; Nicole Abbott[2]; Kasey Hill[2]; Mitch A Phelps[2]; [1]*Sciex, Framingham, MA;* [2]*Ohio State University, Columbus, OH*

ThP 655 **Determination of Plasma Free Amino Acids in Biological Samples using Liquid Chromatography-Tandem Mass Spectrometry**; Jaeman Byun[1]; Subramaniam Pennathur[1]; Anna Mathew[1]; [1]*University of Michigan, Ann Arbor, MI*

ThP 656 **High-resolution Quantitative Metabolomics with biocrates' AbsoluteIDQ® p400 HR kit on Thermo Scientific™ Orbitrap Exploris™ Hybrid Mass Spectrometry Platforms**; Guohui Li[1]; Stephen Dearth[2]; Joshua P. Kline[1]; [1]*Thermo Fisher Scientific – 355 River Oaks Pkwy, San Jose, California;* [2]*biocrates life sciences ag – Eduard-Bodem-Gasse 8, Innsbruck, Austria*

ThP 657 **Metabolomics Changes Associated with the Development and Progression of Parkinson's Disease Identified Through Parallel Reaction Monitoring LC-MS/MS**; Odunayo O. Oluokun[1]; Oluwatosin E. Daramola[1]; Judith Nwaiwu[1]; Mojibola Fowowe[1]; Andrew I. Bennett[1]; Alexandra Lux[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

ThP 658 **Targeted Metabolomic Analysis: Discriminating Hybrid and Wild Hippeastrum Species (Amaryllidaceae) through Alkaloid Profiling by LC-ESI(±)LTQ MS**; Amanda Eiriz Feu[1]; Marcos Valério Vieira Lyrio[1]; Wanderson Romão[1]; Warley de Souza Borges[1]; *[1]UFES, Vitória, Brazil*

ThP 659 **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[1]; Craig Knisley[1]; Timothy Kassis[1]; Mimoun Cadosch Delmar[1]; Lucas Reger[2]; Julia Niemann[2]; David Pollard[2]; Joshua D. Lauterbach[1]; Luke S Ferro[1]; Steven B Hooper[1]; Jack Howland[1]; Jefferson G. Pruyne[1]; Jennifer M Campbell[1]; Jack Geremia[1]; *[1]Matterworks, Inc., Somerville, MA; [2]Sartorius Stedim Biotech GmbH, Goettingen, Germany*

ThP 660 **Pushing the boundaries of speed in Metabolomics: coupling microfluidic capillary electrophoresis with the new ultrafast hybrid nominal mass instrument**; Cristina C. Jacob[1]; Charles Maxey[1]; Philip M. Remes[1]; J. Will Thompson[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]908 Devices Inc., Morrisville, NC*

ThP 661 **A fast and robust LC-MS method for the analysis of basal metabolism in multiple mammalian tissues**; Haiyan Ke[1, 2]; Poonamjot Deol[1]; Manhoi Hur[1, 2]; John Leano[1]; Frances Sladek[1]; Amancio J De Souza[1, 2]; *[1]University of California Riverside, Riverside, CA; [2]UCR Metabolomics Core, University of California, Riverside, California*

ThP 662 **Identification and quantification of cyclic dipeptides in human serum using mass spectrometry**; Anthony Haag[1]; Kathleen Hoch[1]; Sigmund Haidacher[1]; Nian Liu[1]; Tor Savidge[1]; *[1]Baylor College of Medicine, Houston, Texas*

ThP 663 **Intra-laboratory validation of four LC/MS quantitative analytical methods for human plasma metabolomics data integration**; Yuri Imado[1]; Masatomo Takahashi[1, 2]; Yuki Soma[3]; Kohta Nakatani[1, 2]; Taizo Hanai[3]; Yoshihiro Izumi[1, 2]; Takeshi Bamba[1, 2]; *[1]Graduate School of Systems Life Sciences, Kyushu University, Fukuoka, Japan; [2]Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; [3]Graduate School of Bioresource and Bioenvironmental Sciences, Kyushu University, Fukuoka, Japan*

ThP 664 **International ring trial of a standardized quantitative assay analyzing more than 1,000 metabolites across eleven laboratories and seven LC-MS platforms**; Markus Langsdorf[1]; Gregor Ömer[1]; Cornelia Röhring[1]; Tuan Hai Pham[1]; *[1]biocrates life sciences ag, Innsbruck, Austria*

ThP 665 **Urinary metabolomics profiling across mass spectrometer platforms using optimized, matrix-specific calibration standards, quality controls, and acquisition methods**; Gregor Ömer[1]; Markus Langsdorf[1]; Stephen Dearth[1]; *[1]biocrates life sciences ag, Innsbruck, Austria*

ThP 666 **Short Chain Fatty Acid Quantification: Standard Curve or Ratio Quantification?**; Aryeh Korman[1]; Rebecca Jones[1]; Supinda Bunyavanich[2]; Drew R. Jones[1]; *[1]NYU Langone, New York, NY; [2]Icahn School of Medicine at Mount Sinai, New York, NY*

ThP 667 **Towards the understanding of lactate accumulation with CHO cell culture metabolite profiling**; Bo Zhai[1]; Elsa Gorre[1]; Kathryn Dorst[1]; Christopher Sauer[1]; Hirsh Nanda[1]; *[1]Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania*

ThP 668 **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[1]; Daniel Crooks[1]; Laura S. Schmidt[1, 2]; Christopher J. Ricketts[1]; Nunziata Maio[3]; Ronald Holewinski[4]; Thorkell Andresson[4]; Richard Higashi[5]; Teresa W.-M. Fan[5]; Andrew Lane[5]; Youfeng Yang[1]; Cathy C. Vocke[1]; W. Marston Linehan[1]; *[1]Urologic Oncology Branch, Center for Cancer Research, National Cancer Institute, National Institutes of Health, Bethesda, MD; [2]Basic Science Program, Frederick National Laboratory for Cancer Research, National Cancer Institute, Frederick, MD; [3]Section on Cell Biology and Metabolism, Eunice Kennedy Shriver National Institute of Child Health and Human Development, National Institutes of Health, Bethesda, MD; [4]Leidos Biomedical Research, Inc., Frederick National Laboratory for Cancer Research, National Cancer Institute, Bethesda, MD; [5]Department of Toxicology and Cancer Biology, Markey Cancer Center, University of Kentucky, Lexington, KY*

ThP 669 **Efficient and Improved LC-MS/MS Quantitation of Phenolic Acids and Lignans from Human Fecal Samples**; Chris Dickson[1]; Jonathan Rickmeyer[2]; Felix Grun[2]; Elizabeth Bess[2]; *[1]University of California Irvine, Irvine, CA; [2]University of California, Irvine, Irvine, CA*

ThP 670 **In vivostable isotope tracing and metabolomics for the identification of synthetically lethal metabolic vulnerabilities in glioblastomas**; Suresh Udutha[1]; Céline Taglang[1]; Georgios Batsios[1]; Anne Marie Gillespie[1]; Meryssa Tran[1]; Pavithra Viswanath[1]; *[1]UCSF, San Francisco, CA*

ThP 671 **Development of a Simultaneous Quantitation and Discovery (SQUAD) workflow for coeluting sugar-phosphates using orthogonal fragmentation techniques**; Sunandini Yedla[1]; Brandon Bills[1]; Rahul Deshpande[1]; Bashar Amer[1]; Susan S Bird[1]; Vlad Zabrouskov[1]; *[1]ThermoFisher Scientific, San Jose, CA*

ThP 672 **Development and Evaluation of a Fast LC-MS Assay to Quantify NAD-Associated Metabolites in Cancer Cells**; Mike Lingjue Wang[1]; Ryan Conrad[1]; Scott Foster[1]; Dewakar Sangaraju[1]; Xiaorong Liang[1]; Brian Dean[1]; Zijuan Lai[1]; *[1]Genentech Inc., South San Francisco, CA*

NATURAL PRODUCTS
673-700

ThP 673 **The membrane protein Rv2113 is crucial for the anti-tubercular activity of Callyaerins**; David Podlesainski[1]; Emmanuel Tola Adeniyi[2]; Violetta Krisilia[2]; Florian Schulz[1]; Tim Richter[1]; Farnusch Kaschani[1]; Rainer Kalscheuer[2]; Markus Kaiser[1]; *[1]University Duisburg-Essen, Essen, Germany; [2]Heinrich Heine University, Düsseldorf, Germany*

ThP 674 **Rationally Minimizing Natural Product Libraries without Chemical Diversity Sacrifice using Untargeted Metabolomics**; Monica Ness[1, 2]; Thilini Peramuna[1]; Karen Wendt[1]; Crystal Okeke[1]; Robert H Cichewicz[1]; Laura-Isobel McCall[1, 2]; *[1]University of Oklahoma, Norman, OK; [2]San Diego State University, San Diego, CA*

ThP 675 **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[1]; Bernd Steklis[1]; Tyler Arntz[1]; Todd Blackledge[1]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH*

ThP 676 **Bridging the Gap: A Comparative Analysis of Orbitrap and Ion Cyclotron Resonance Mass Spectrometers on Natural Organic Matter**; Charlotte Brun[1]; Mourad Harir[2]; Christos Panagiotopoulos[3]; Philippe Schmitt-Kopplin[2, 4]; Sébastien Schramm[5]; Maxime Bridoux[1]; *[1]CEA, DAM, DIF, F-91297, Arpajon, France; [2]Research Unit Analytical BioGeoChemistry, Helmholt Munich, 85764 Neuherberg, Germany; [3]M.I.O. Institut Méditerranéen d'Océanologie, Aix Marseille Univ., Université de Toulon, CNRS, IRD, F-13288, Marseille, France; [4]Analytical Food Chemistry, TUM, Maximus-von-Imhof-Forum 2, 85354 Freising, Germany; [5]Laboratoire de Chimie et de Physique – Approches Multi-échelles des Milieux Complexes (LCP-A2MC), Université de Lorraine, F-57078, Metz, France*

ThP 677 **Influence of Geographic Variation on Chemistry and Metabolomics of Pacific Northwest Endemic Lobaria sp. Cyanolichens**; Xinhui Yu[1]; Wilmer Perera[2]; Joseph Di Meglio[3]; Bruce McCune[3]; Kerry McPhail[3]; *[1]Oregon State University, Corvallis, OR; [2]CAMAG Scientific,, Wilmington, NC; [3]Oregon State University, Corvallis, Oregon*

ThP 678 **In-depth characterization and structure elucidation of non-ribosomal peptides related to adenopeptin using LC-HRAM-MSn**; Douglas Marchbank[1]; Sven Hackbusch[2]; Bradley Haltli[1]; Brandon Bills[3]; Min Du[4]; [1]*Croda Canada Ltd, Charlottetown, PEI;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*ThermoFisher Scientific, San Jose, CA;* [4]*Thermo Fisher Scientific, Lexington, MA*

ThP 679 **Identification of antimicrobial peptides against bacterium Burkholderia glumae**; Jeffrey Ocampo[1]; Leslie M. Hicks[1]; [1]*University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 680 **Investigation of the Underlying Mechanism of Lasso Peptide Thermal Unthreading using LC-TIMS-q-ECD ToF MS/MS**; Kevin Jeanne Dit Fouque[1]; Miguel Santos[1]; Negin Asgharihosseinpour[2]; Severine Zirah[3]; Julian D Hegemann[2]; Francisco A Fernandez-Lima[1]; [1]*Florida International University, Miami, FL;* [2]*Saarland University, Saarbrücken, Germany;* [3]*National Museum of Natural History, Paris, France*

ThP 681 **Induction of Plant Bioactive Peptides in Response to Environmental Stressors**; Katelyn D Wix[1]; Leslie M. Hicks[1]; [1]*University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 682 **Characterization of the lasso and branched-cyclic Syanodin I using Hydrogen-Deuterium Exchange, Trapped Ion Mobility Spectrometry, and tandem ECD-MS/MS**; Miguel Santos[1]; Kevin Jeanne Dit Fouque[1]; Ukesh Karki[1]; Julian D Hegemann[2]; Prem Chapagain[1]; Francisco A Fernandez-Lima[1]; [1]*Florida International University, Miami, FL;* [2]*Helmholtz Institute for Pharmaceutical Research Saarland (HIPS), Helmholtz Centre for Infection Research, Saarbrücken, Germany*

ThP 683 **Assessing biological and metabolic diversity in Trichodermafor natural product library assembly using untargeted metabolomics**; Thilini Peramuna[1]; Monica Ness[1, 2]; Karen Wendt[1]; Robert H Cichewicz[1]; Laura-Isobel McCall[2]; [1]*University of Oklahoma, Norman, OK;* [2]*San Diego State University, San Diego, CA*

ThP 684 **Determination of cycloastragenol in dietary supplements containing the adaptogenic herb Astragalus trimestris using HPLC-MS/MS**; Katerina Knizkova[1]; Martin Kuchar[1]; Petra Cihlarova[1]; [1]*Forensic Laboratory of Biologically Active Substances, Department of Chemistry of Natural Compounds, University of Chemistry and Technology, Prague, Czech Republic*

ThP 685 **Determination of 2-phenoxychromones and structurally related flavonols using LC–QTOF tandem mass spectrometry combined with molecular networking analysis**; In Jin Ha[1, 2]; Min Young Lee[1]; Seok-Geun Lee[1, 2]; Kwang Seok Ahn[2]; Junhee Lee[1, 2]; [1]*Kyung Hee University Korean Medicine Hospital, Seoul, South Korea;* [2]*College of Korean Medicine, Kyung Hee University, Seoul, South Korea*

ThP 686 **A rapid method to differentiate and identify isomers of A-type procyanidins**; Pai-Chi Syue[1]; Kuok Fai Li[1]; Kuo-Lung Ku[1]; Yao-Yuan Chuang[2]; [1]*National Chiayi University, Chiayi City, Taiwan;* [2]*National University of Kaohsiung, Kaohsiung City, Taiwan*

ThP 687 **Detection of Upregulation and Downregulation of Fungal Secondary Metabolism from Penicillium spp by Liquid Microjunction Surface Sampling Probe (LMJSSP)**; Jessie F. Deng[1]; Jennifer L. Kolwich[1]; Haidy Metwally[1]; Georgia Reed[2]; Randy E. Ellis[2, 3, 4, 5]; Avena C. Ross[1]; Richard D. Oleschuk[1]; [1]*Department of Chemistry, Queen's University, Kingston, ON;* [2]*School of Computing, Queen's University, Kingston, ON;* [3]*Department of Mechanical and Materials Engineering, Queen's University, Kingston, ON;* [4]*Department of Surgery, Queen's University, Kingston, ON;* [5]*Department of Biomedical and Molecular Sciences, Queen's University, Kingston, ON*

ThP 688 **Mapping Metabolite Dynamics of Soil Microbe Interactions using a Liquid Microjunction Surface Sampling Probe (LMJSSP)**; Jennifer L. Kolwich[1]; Lainey K. Ennett[1]; Jessie F. Deng[1]; Richard D. Oleschuk[1]; Avena C. Ross[1]; [1]*Queen's University, Kingston, ON*

ThP 689 **UHPLC-MS/MS profiling of alkaloids in opium and poppy straw**; Petra Cihlarova[1]; Viktorie Lukesova[1]; Katerina Knizkova[1]; Martin Kuchar[1]; [1]*Forensic Laboratory of Biologically Active Substances, Department of Chemistry of Natural Compounds, University of Chemistry and Technology, Prague, Czech Republic*

ThP 690 **Use of IMS HDMSe for the Analysis of Anthocyanins, Procyanidins and Other Flavonoids in Food and Natural Product Samples**; Gordon T Fujimoto[1]; Lindsay E Hatch[1]; Sarah E Dowd[1]; Emily R Britton[1]; [1]*Waters Corporation, Milford, Massachusetts*

ThP 691 **Development of a novel non-targeted method for authentication of American ginseng using ASAP-MS and UPLC-QTOF-MS**; Sanem Hosbas Coskun[1, 2]; Aaron A. Urbas[2]; Adam J. Kuszak[1]; Aysel Berkkan[2, 3]; Benjamin J. Place[2]; Catherine A. Rimmer[2]; David A. Sheen[2]; [1]*Office of Dietary Supplements, National Institutes of Health, Bethesda, MD;* [2]*National Institute of Standards and Technology, Gaithersburg, MD;* [3]*Gazi University Faculty of Pharmacy Department of Analytical Chemistry, Ankara, Turkey*

ThP 692 **Knowledge-based data strategies bridge the gap for automated data analysisof phytochemical diversity in Withania somnifera**; Rudranil Dutta[1, 2]; Luke C Marney[1, 2]; Jaewoo Choi[1, 2]; Liping Yang[1, 2]; Amala Soumyanath[2, 3]; Jan F. Stevens[2, 4, 5]; Claudia S. Maier[1, 2, 4]; [1]*Department of Chemistry, Oregon State University, Corvallis, OR;* [2]*BENFRA Botanical Dietary Supplements Research Center, Oregon Health and Science University, Portland, OR;* [3]*Department of Neurology, Oregon Health and Science University, Portland, Oregon;* [4]*Linus Pauling Institute, Oregon State University, Corvallis, OR;* [5]*Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR*

ThP 693 **Mass Spectrometric Analysis of Antifungal Secondary Metabolites of a Streptomyces murinus Isolate from Vietnam**; Cloe R Zimmerman[1, 2]; Thi Thuy Tien Nguyen[3]; Lauren Konig[1, 4]; Karine Bagramyan[1]; Markus Kalkum[1, 2]; [1]*Department of Immunology and Theranostics, City of Hope, Duarte, CA;* [2]*Irell & Manella Graduate School of Biological Sciences, City of Hope, Duarte, CA;* [3]*Department of Engineering and Food Technology, University of Agriculture and Forestry, Hue University, Hue City, Vietnam;* [4]*Indiana University Bloomington, Bloomington, IN*

ThP 694 **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[1, 2]; Vera Alenicheva[1, 2]; Bailey Keefe[3]; Jaewoo Choi[1, 2]; Liping Yang[1, 2]; Nora Gray[2, 4]; Amala Soumyanath[2, 4]; Kevin Brown[2, 3, 5]; Jan F. Stevens[2, 3, 6]; Claudia S. Maier[1, 2, 6]; [1]*Department of Chemistry, Oregon State University, Corvallis, OR;* [2]*BENFRA Botanical Dietary Supplements Research Center, Oregon Health and Science University, Portland, OR;* [3]*Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR;* [4]*Department of Neurology, Oregon Health and Science University, Portland, Oregon;* [5]*School of Chemical, Biological, and Environmental Engineering, Oregon State University, Corvallis, Oregon;* [6]*Linus Pauling Institute, Oregon State University, Corvallis, OR*

ThP 695 **HRAM analysis and spectral data mining of museum-sourced cnidarian extracts for natural product investigations**; Jennifer E Netjes[1]; Sam Afoullouss[1]; Dale Chaput[1]; Andrea Quattrini[2]; Bill Baker[1]; [1]*University of South Florida, Tampa, FL;* [2]*National Museum of Natural History, Smithsonian Institution, Washington, DC*

ThP 696 **Molecular network guided isolation of new aphrocallistin for deep-sea sponge Aphrocallistes sp enhanced by Ion Mobility.**; Sam Afoullouss[1]; Jennifer Netjes[1]; Ryan M. Young[2]; Fred Valeriote[3]; Mark P. Johnson[2]; A. Louise Allcock[2]; BIll J. Baker[1]; [1]*University of South Florida, Tampa, FL;* [2]*Ryan Institute & School of Natural Sciences, University* *of Galway, University Road, Galway, Ireland, Galway, Ireland; [3]Department of Internal Medicine, Division of Hematology and Oncology, Henry Ford Hospital,, Detroit, MI*

ThP 697 **Comparison of nocturnal and diurnal metabolomes of rose flowers and leaves**; Julie Zumsteg[1]; Elodie Bossard[2]; Lorène Gourguillon[2]; Claire Villette[1]; Dimitri Heintz[1]; *[1]CNRS IBMP, Strasbourg, France; [2]Advanced Biobased and Bioinspired Ingredients, LVMH Recherche, Saint-Jean-de-Braye, France*

ThP 698 **Towards the isolation of traditionally utilized plant-origin antiparasitic compounds through chemometrics-guided serial fractionation and in vitro assay**; Grace Ochigbo[1]; Brenda Holder[2]; Ralph Hindle[3]; Kathy Hunt[3]; James D Wasmuth[1]; Brielle V Rosa[1]; *[1]University of Calgary, Faculty of Veterinary Medicine, Calgary, AB; [2]Cree Traditional Knowledge Keeper, Jasper National Park, AB; [3]Vogon Laboratory Services Ltd., Cochrane, AB*

ThP 699 **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[1]; David E Alonso[1]; John Hayes[1]; Joseph E Binkley[1]; *[1]LECO Corporation, Saint Joseph, MI*

ThP 700 **Automation of QuEChERS extraction for quantitation of CBD and THC in cannabis leaves in 8 seconds per sample**; Jonathan Rochon[1]; Serge Auger[1]; Mégane Moreau[1]; Sarah Demers[1]; Jean Lacoursière[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Inc., Quebec, QC*

PROTEINS: PTMS II
701-721

ThP 701 **Discovery of omega-3 polyunsaturated fat-derived lysine iminylation as a novel, chemically labile post-translational modification**; Bingsen Zhang[1, 2]; Frank C Schroeder[1, 2]; *[1]Cornell University, Ithaca, NY; [2]Boyce Thompson Institute, Ithaca, NY*

ThP 702 **Capturing the polyUbiquitylome with pUb-STRACTER (Stringent Trypsin-Resistant Affinity Capture with Targeted Enzymatic Recovery)**; Harvey E. Johnston[1]; Rahul S. Samant[1]; *[1]Babraham Institute, Cambridge, United Kingdom*

ThP 703 **Re-exploring Zirconia Chromatography to Enhance Phosphoproteome Coverage**; Kosuke Ogata[1]; Naoyuki Sugiyama[1]; Yasushi Ishihama[1, 2]; *[1]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; [2]National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan*

ThP 704 **-Exploring the role of reversible cysteine oxidation in tardigrade osmobiosis**; Samantha J Balboa[1]; Evan R. Stair[1]; Meredith H. Daughtridge[1]; Abel A. Salas[1]; Brendin Flinn[2]; Derrick Kolling[2]; Leslie M. Hicks[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Marshall University, Huntington, West Virginia*

ThP 705 **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[1]; Haichuan Liu[2]; Marcia Santos[3]; Rashmi Madda[2]; Jingwen Ding[4]; Scott Mack[4]; Maggie Ostrowski[4]; Elliott Jones[2]; Paul Clemens[2]; *[1]Sciex, Redwood City, CA; [2]SCIEX, Redwood City, CA; [3]SCIEX, Brea,, CA; [4]SCIEX, Fremont, CA*

ThP 706 **Short-chain fatty acids propionate and butyrate control growth and differentiation linked to cellular metabolism**; Michael Nshanian[1]; Benjamin S. Geller[1]; Joshua J. Gruber[1]; Faye Chleilat[1]; Jeannie Marie Camarillo[2]; Neil L. Kelleher[2, 3]; Yingming Zhao[4]; Michael P. Snyder[1, 5]; *[1]Department of Genetics, Stanford University School of Medicine, Stanford, CA; [2]Department of Chemistry, Molecular Biosciences and Proteomics Center of Excellence, Northwestern University, Evanston, IL; [3]Department of Biochemistry and Molecular Genetics, Feinberg School of Medicine, Northwestern University, Evanston, IL; [4]Ben May Department of Cancer Research Committee on Cancer Biology, University of Chicago, Chicago, IL; [5]Center for Genomics and Personalized Medicine, Stanford University School of Medicine, Stanford, CA*

ThP 707 **DISCOVERY OF A NOVEL ITACONATE-MEDIATED METHYLSUCCINYLATION**; Dongyang Liu[1]; Chu Wang[1]; *[1]Peking University, Beijing, China*

ThP 708 **Methionine alkylation as an approach to quantify methionine oxidation using mass spectrometry**; Margaret M Hoare[1]; Ruiyue Tan[1]; Kevin A Welle[2]; Kyle Swovick[2]; Jennifer R Hryhorenko[2]; Sina Ghaemmaghami[1, 2]; *[1]University of Rochester, Rochester, NY; [2]University of Rochester Mass Spectrometry Resource Laboratory, Rochester, NY*

ThP 709 **Investigating the self-pupylation of PafA in the Pup-proteasome system**; Jacquelyn C Ogata-Bean[1]; Alicia Plourde[1]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON*

ThP 710 **Genotype-dependent N-glycosylation and novel O-glycosylation affect the activation of histidine-rich glycoprotein by plasmin**; Yang Zou[1, 2]; Matti F. Pronker[1, 2]; Karli R. Reiding[1, 2]; Albert J.R. Heck[1, 2]; *[1]Utrecht University, Utrecht, Netherlands; [2]Netherlands Proteomics Center, Utrecht, Netherlands*

ThP 711 **Quantification of ADP-ribosylated proteins in neutrophils using an Orbitrap Astral mass spectrometer**; Hayoung Cho[1]; Ivo A Hendriks[1]; Michael L Nielsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark*

ThP 712 **Multiplexed ubiquitome profiling in dozens of cell levels without enrichment using a boosting channel**; Minsang Hwang[1, 2]; Jong-Seo Kim[1, 2]; *[1]School of Biological Sciences, Seoul National University, Seoul, South Korea; [2]Center for RNA Research, Institute of Basic Science (IBS), Seoul, South Korea*

ThP 713 **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[1]; Meeli Mullari[1]; Hayoung Cho[1]; Aurél G. Prósz[2]; Sara C. Buch-Larsen[1]; Marie Locard-Paulet[3]; Zoltan Szallasi[2, 4]; Michael L Nielsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, Proteomics Program, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; [2]Danish Cancer Institute, Copenhagen, Denmark; [3]Institut de Pharmacologie et de Biologie Structurale (IPBS), Université de Toulouse, CNRS, Université Toulouse III - Paul Sabatier (UT3), Toulouse, France; [4]Computational Health Informatics Program, Boston Children's Hospital, Boston, MA*

ThP 714 **Optimal Dissociation Methods for Enhancing Identification and Quantitative Accuracy of Various Glycan Types in Intact N-glycopeptides Analysis**; Zhenyu Sun[1]; Yingwei Hu[1]; T. Mamie Lih[1]; Jongmin Woo[1]; Hui Zhang[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

ThP 715 **Bottom-Up, Middle-Down, or Top-Down Collision Induced Dissociation? Pros and Cons for Retaining and Localizing Labile Post-Translational Modifications**; Neven N. Mikawy[1]; Kristina Hakansson[1]; *[1]University of Michigan Department of Chemistry, Ann Arbor, MI*

ThP 716 **Profiling Protein Post-Translational Modifications in Plasma-derived Extracellular Vesicles as Fingerprints for Breast Cancer Subtypes**; Marco Hadisurya[1]; Hillary Andaluz Aguilar[2]; Mengting Xu[3]; I-Hsuan Chen[1]; J. Sebastian Paez[4]; Zheng-Chi Lee[1, 5]; Anton B. Iliuk[6]; Sonia Sugg[7]; Weizhou Zhang[8]; W. Andy Tao[1, 2, 4, 9]; *[1]Department of Biochemistry, Purdue University, West Lafayette, IN; [2]Department of Chemistry, Purdue University, West Lafayette, IN; [3]School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN; [4]Department of Medical Chemistry and Molecular Pharmacology, Purdue University, West Lafayette, IN; [5]West Lafayette Junior/Senior High School, West Lafayette, IN; [6]Tymora Analytical Operations, West Lafayette, IN; [7]College* *of Medicine, University of Iowa, Iowa City, IW; [8]College of Medicine, University of Florida, Gainesville, FL; [9]Purdue Institute for Cancer Research, Purdue University, West Lafayette, IN*

ThP 717 **Identification of isoaspartic acid residues in proteins by deuterium labeling and mass spectrometry**; Masaru Miyagi[1]; Kelao Neumbo[2]; Takashi Nakazawa[3]; *[1]Case Western Reserve Univers, Cleveland, OH; [2]Case Western Reserve University, Cleveland, OH; [3]Nara Women's University, Nara, Japan*

ThP 718 **A Systematic Investigation of Citrullination and Corresponding Structural Effect in Human Rheumatoid Arthritis**; Zexin Zhu[1]; Wei Li[2]; Hung-Yu (Eric) Chiang[3]; Hua Zhang[2]; Zhicheng Jin[4]; Lingjun Li[2]; *[1]University of Wisconsin - Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Department of Biophysics, University of Wisconsin-Madison, Madison, WI; [4]Department of Pathology and Laboratory Medicine, University of Wisconsin-Madison, Madison, WI*

ThP 719 **Acetylation of RORβ DNA binding domain and hinge region by histone acetyltransferase p300 modulates RORβ stability and transactivation**; Timothy R O'Leary[1]; Ruben D. Garcia-Ordonez[1]; Patrick R. Griffin[1]; Mi Ra Chang[1]; *[1]UF Scripps, Florida, Jupiter, FL*

ThP 720 **Lysine lactylation controls liquid-liquid phase separation and immune signaling during viral infection**; Matthew D Tyl[1]; Victoria Merengwa[1]; Ileana M Cristea[1]; *[1]Princeton University, Princeton, NJ*

ThP 721 **Systematic investigation of the N-terminal effect on protein stability**; Zeyu Wang[1]; Senhan Xu[1]; Kejun Yin[1]; Xing Xu[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

PROTEOMICS: CLINICAL APPLICATIONS II
722-743

ThP 722 **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[1]; Nikki Atwal[1]; Lee A Gethings[1]; Christopher J Hughes[1]; Richard Lock[1]; Nelofor Syed[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Imperial College London, London, United Kingdom*

ThP 723 **The Impact of Maternal Vitamin D Status during Breastfeeding on Human Milk Proteome**; Rony Hull[1]; Jennifer R Bethard[1]; John E Baatz[1]; Katherine Chetta[1]; Danforth A Newton[1]; Carol L Wagner[1]; Lauren E Ball[1]; *[1]Medical University of South Carolina, Charleston, SC*

ThP 724 **Refining Classification of Cholangiocarcinoma Subtypes via Proteogenomic Integration Reveals New Therapeutic Prospects**; Heeyoun Hwang; *Korea Basic Science Institute, cheongju, South Korea*

ThP 725 **Enhanced Detection of Hemoglobin Variants in Clinical Research using Dried Blood Spot and High-Resolution, Accurate-Mass (HRAM) MS**; Yvonne Ehwang Song[1]; Kerry Hassell[1]; Edward Goucher[2]; Jingshu Guo[1]; Tanis Correa[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*

ThP 726 **An Interlaboratory Comparison of a Highly Multiplexed, Quantitative Peptide Assay to Measure Health Surveillance Panel Proteins in Plasma**; Chi D. L. Nguyen[1]; Matthew Daly[2]; Lee Gethings[2]; Jennifer E. Van Eyk[3]; Susan M. Mockus[4]; *[1]Precision Biomarker Laboratories, Cedars Sinai Medical Center, Beverly Hills, CA; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Advanced Clinical BioSystems Research Institute, Cedars-Sinai Medical Center, Los Angeles, California; [4]Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, California*

ThP 727 **High-throughput platelet proteomics from small amounts of previously frozen samples adds another layer to plasma-based immunophenotyping**; Dylan Nicholas T Tabang[1]; Kathrin Korff[1, 2]; Kaitlin Brannon[1]; Komal Mandal[1]; Julia Tilburg[3, 4]; Patrick Van Zalm[1]; Arthur Viodé[1]; Arjun Ravishankar[5]; Jin Gyu Cheong[5]; Steven Z Josefowicz[5]; Joseph E Italiano[3, 4]; Kinga K Smolen[6, 7]; Hanno Steen[1, 7]; *[1]Department of Pathology, Boston Children's Hospital and Harvard Medical School, Boston, MA; [2]Faculty of Chemistry, Aalen University, Aalen, Germany; [3]Department of Surgery, Harvard Medical School, Boston, MA; [4]Vascular Biology Program, Boston Children's Hospital, Boston, MA; [5]Laboratory of Epigenetics and Immunity, Department of Pathology and Laboratory Medicine, Weill Cornell Medicine, New York, NY; [6]Department of Pediatrics, Boston Children's Hospital and Harvard Medical School, Boston, MA; [7]Precision Vaccines Program, Division of Infectious Diseases, Boston Children's Hospital, Boston, MA*

ThP 728 **Multiple reaction monitoring-mass spectrometry-based assay for nondepleted plasma protein quantitation: Application to screening for psychiatric disorders**; Dongyoon Shin[1]; Yeongshin Kim[2]; Junho Park[1, 3]; Youngsoo Kim[1, 2]; *[1]Proteomics Research Team, CHA Institute of Future Medicine, Pangyo, South Korea; [2]Department of Medical Science, School of Medicine, CHA University, Pangyo, South Korea; [3]Department of Pharmacology, School of Medicine, CHA University, Pangyo, South Korea*

ThP 729 **Analysis of HMGB1 protein secreted by lung and colon cancer cells in response to oxaliplatin**; Jingqi Fan[1]; Kevin P. Gillespie[1]; Clementina Mesaros[1]; Ian Alexander Blair[1]; *[1]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*

ThP 730 **High sensitivity measurement of CSF and plasma tau phosphorylation in Alzheimer's disease using Orbitrap Astral mass spectrometer**; Joanna M Kirkpatrick[1]; Laia Montoliu-Gaya[2]; Gunnar Brinkmalm[2]; Eugen Damoc[3]; Tabiwang N Arrey[3]; Bernard Delanghe[3]; Kaj Blennow[2]; Henrik Zetterberg[2]; Johan Gobom[2]; *[1]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [2]Institute of Neuroscience and Physiology, University of Gothenburg, Neurochemistry laboratory SU/Mölndal Hospital, Mölndal, Sweden; [3]Thermo Fisher Scientific, Bremen, Germany*

ThP 731 **Absolute quantification of BRCA1 protein levels in formalin-fixed, paraffin-embedded (FFPE) tissue by FAIMS-PRM**; Beom-Jun Kim[1]; Steve M. Sweet[1]; Camille Lombard-Banek[1]; David C. Chain[1]; Josep V. Forment[2]; Natalia Lukashchuk[2]; Yeoun Jin Kim[1]; *[1]AstraZeneca, Gaithersburg, MD; [2]AstraZeneca, Cambridge, United Kingdom*

ThP 732 **Serum Proteome Profiling of Diabetic Patients Treated with Novel Antidiabetics Shows Improved Cognitive Function, Cardiovascular Function, and Reduce Inflammatory Responses**; Md Abdul Hakim[1]; Shams Osman[2]; Akeem Sanni[1]; Waziha Purba[1]; Md Mostofa Al Amin Bhuiyan[1]; Sherifdeen Onigbinde[1]; Arvin Saffarian Delkhosh[1]; Ahmed El-Yazbi[3]; Yehia Mechref[1]; *[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; [2]Department of Clinical Pharmacy and Pharmacy Practice, Faculty of Pharmacy, Alexandria University, Alexandria, Egypt; [3]Department of Pharmacology and Therapeutics, Faculty of Pharmacy, Alamein International University, Alamein, Egypt*

ThP 733 **Exploring the Impact of Fasting on Biological Pathways through LC-MS/MS of Profiling Serum Proteome**; Md Mostofa Al Amin Bhuiyan[1]; Waziha Purba[1]; Md Abdul Hakim[1]; Ayobami Oluokun[1]; Ahmed Elyazbi[2]; Haneen S. Dwaib[3]; Yehia Mechref[1]; *[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; [2]Department of Pharmacology and Therapeutics, Faculty of Pharmacy, Alamein International University, Alamein, Egypt; [3]Clinical Nutrition Department, Palestine Ahliya University, Bethlehem, Palestine*

ThP 734 **Conventional anticoagulants allow preanalytical variation that confounds the accuracy of plasma proteomics**; Rachel M Miller[1]; Sama Mehta[1]; Xiaoyuan Zhou[2]; Nicholas Mucci[2]; Ryan W. Benz[2]; Jing Li[1]; *[1]Streck LLC., La Vista, NE; [2]Seer Inc., Redwood City, CA*

ThP 735 **Fucoidan ameliorates skin fibrosis via tight junction regulation**; Pang-Hung Hsu; *National Taiwan Ocean University, Keelung, Taiwan*

ThP 736 **Proteome and Tau Profiles in Extracellular Vesicles Derived from Brain Fluid among human tauopathies by mass spectrometry**; Laura Fichter[1]; Elodie Leroux[2]; Marie Oosterlynck[2]; Morvane Colin[2]; Jérôme Vialaret[3]; Sylvain Lehmann[3]; Luc Buée[2]; Christophe Hirtz[3]; [1]*PPC - CHU de Montpellier, Montpellier, France;* [2]*Alzheimer et Tauopathies, Lille Neuroscience & Cognition, Lille, France;* [3]*PPC - CHU de Montpellier, MONTPELLIER, France*

ThP 737 **Identification of blood group variants using RBC ghost membrane proteomics**; Ankit P Jain[1]; Anne Roberts[1]; Lilian R Heil[2]; John D Roback[1,3]; Blaine Roberts[1]; [1]*Emory University School of Medicine, Atlanta, GA;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*Emory University Hospital, Atlanta, GA*

ThP 738 **Efficient Human Plasma Proteome Profiling at up to 300 Samples Per Day**; Paul Jacobs[1]; Jeff Op De Beeck[2]; Robert Van Ling[3]; Yuan Lin[4]; Shanhua Lin[4]; [1]*Thermo Fisher Scientific - Belgium, Ghent, Belgium;* [2]*Thermo Fisher Scientific, Ghent, Belgium;* [3]*Thermo Fisher Scientific - Breda, Breda, Netherlands;* [4]*Thermo Fisher Scientific, Sunnyvale, CA*

ThP 739 **Fast-tracking the journey to targeted clinical assays with a novel hybrid high-speed nominal mass instrument**; Maria Wahle[1]; Vincent Albrecht[1]; Johannes Mueller-Reif[1]; Philip M. Remes[2]; Cristina Jacob[2]; Claudia Martins[2]; Stevan Horning[3]; Matthias Mann[1]; [1]*Department of Proteomics and signal Transduction, Max-Planck-Institute of Biochemistry, Martinsried (near Munich), Germany;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 740 **Merits of bacterial classification with microflow LC-MS/MS**; Miriam Abele[1,2]; Armin Soleymaniniya[3]; Etienne Doll[4]; Siegfried Scherer[4]; Klaus Neuhaus[5]; Nina Wantia[6]; Mathias Wilhelm[3]; Bernhard Kuster[1,2]; Christina Ludwig[1]; [1]*Bavarian Center for Biomolecular Mass Spectrometry, TU Munich, TUM School of Life Sciences, Freising, Germany;* [2]*Chair of Proteomics and Bioanalytics, TU Munich, TUM School of Life Sciences, Freising, Germany;* [3]*Computational Mass Spectrometry, TU Munich, TUM School of Life Sciences, Freising, Germany;* [4]*Chair of Microbial Ecology, TU Munich, TUM School of Life Sciences, Freising, Germany;* [5]*Core Facility Microbiome, ZIEL Institute for Food & Health, TU Munich, Freising, Germany;* [6]*Institut für Medizinische Mikrobiologie, Immunologie und Hygiene, TUM School of Medicine and Health, TU Munich, München, Germany*

ThP 741 **Deep plasma protein profiling enabled by nanoparticle-based sample preparation and Orbitrap Astral mass spectrometer**; William F Beimers[1]; Katherine A Overmyer[1,2,3]; Rachael Wilson[4,5]; Sterling C Johnson[4,5,6]; Joshua J Coon[1,2,3,7]; [1]*Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI;* [2]*Morgridge Institute for Research, Madison, WI;* [3]*National Center for Quantitative Biology of Complex Systems, Madison, WI;* [4]*Wisconsin Alzheimer's Institute, Madison, WI;* [5]*Wisconsin Alzheimer's Disease Research Center, Madison, WI;* [6]*Department of Medicine, University of Wisconsin-Madison, Madison, WI;* [7]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

ThP 742 **Quantification of the PD-1/PD-L1 Axis in Various Cancer Types by Immuno-Multiple Reaction Monitoring**; Neda Boushehri[1,2]; Vincent Lacasse[1,3]; Alan Spatz[3,4]; Robert Popp[5]; Rene P. Zahedi[6,7,8,9]; Kevin Kunhong Xiao[10]; Patrick L. Wagner[10]; Sitara Niranjan[10]; Rachel Dileo[10]; Huseyin Sakib Karakilic[10]; Amanjit Gil[10]; Christoph H. Borchers[1,2,3,4]; [1]*Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC;* [2]*Division of Experimental Medicine, McGill University, Montreal, QC;* [3]*Department of Pathology, McGill University, Montreal, QC;* [4]*Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC;* [5]*MRM Proteomics Inc, Montreal, QC;* [6]*Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB;* [7]*Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB;* [8]*Department of Internal Medicine, University of Manitoba, Winnipeg, MB;* [9]*CancerCare Manitoba Research Institute, Winnipeg, MB;* [10]*Allegheny Health Network Cancer Institute, Pittsburgh, PA*

ThP 743 **A large-scale DIA-MS acquisition of iPSC-derived motor neurons**; Oliver Y Wang[1]; Oleg A. Karpov[1]; Niveda Sundararaman[1]; Rakhi Pandey[1]; Velina Kozareva[2]; Stanislav Tsitkov[2]; Dhruv Sareen[1]; Ernest Fraenkel[2]; Clive Svendsen[1]; Jennifer E. Van Eyk[1]; [1]*Cedars-Sinai Medical Center, Los Angeles, CA;* [2]*Massachusetts Institute of Technology, Cambridge, MA*

PROTEOMICS: INTACT PROTEINS AND TOP DOWN ANALYSIS II
744-772

ThP 744 **Combinatorial Probabilities of Multiple Fragmentations Explain Polypeptide MS/MS Intensity Distribution, Overrepresentation of Smaller Fragments, and Missing Middle of Top-Down MS**; Wensheng Yang[1]; Novera Alam[1]; Jeffrey Agar[1]; [1]*Northeastern University, Boston, MA*

ThP 745 **Optimization of TDMS analysis of proteoforms from membrane-bound particles for future translational studies based on human plasma**; Amal Mohamed Kamal Eltobshi[1]; Jake Kline[1]; Luca Fornelli[1]; [1]*University of Oklahoma, Norman, OK*

ThP 746 **Fast and Robust Proteoforms Platform Development via Immunoaffinity Purifications Coupling to Top-Down Mass Spectrometry (IP-MS) for Biomarkers Precision Medicine**; Nadia Sultana[1]; Baoliang Cui[1]; Khader Awwad[1]; Michael Schulz[1]; Qin Ji[1]; Mario Richter[1]; Yu Tian[1]; [1]*Research & Development, AbbVie, North Chicago, IL*

ThP 747 **Evaluation of Intact Protein Extraction Strategies in Top-Down Proteomics**; Xingzhao Xiong[1]; Xiaowen Liu[1]; [1]*Tulane University, New Orleans, LA*

ThP 748 **Deep Profiling of Plasma Proteoforms with Engineered Nanoparticles for Top-down Proteomics Analysis**; Che-Fan Huang[1]; Aniel Sanchez[1]; Mrittika Bhattacharya[2]; Giang Ho[2]; Ambika Sundaresan[2]; Michael A. Hollas[1]; Michael A. Caldwell[1]; Xiaoyan Zhao[2]; Ryan W. Benz[2]; Asim Siddiqui[2]; Neil L. Kelleher[1]; [1]*Northwestern University, Evanston, IL;* [2]*Seer Inc., Redwood City, CA*

ThP 749 **Demultiplexing of Top-down Data-Dependent Acquisition Mass Spectrometry**; Zhige Wang[1]; Xingzhao Xiong[1]; Xiaowen Liu[1]; [1]*Tulane University, New Orleans, LA*

ThP 750 **Developing Advanced Capillary Zone Electrophoresis-Mass Spectrometry Techniques for Multi-Level Proteomics of Complex Biological Samples**; Qianyi Wang[1]; Qianjie Wang[1]; Zihao Qi[2]; William Moeller[2]; Shaolei Lu[3]; Xiaowen Liu[4]; Chiung-Kuei Huang[4]; Vicki Wysocki[2]; Liangliang Sun[1]; [1]*Michigan State University, East Lansing, MI;* [2]*Ohio State University, Columbus, OH;* [3]*Brown University, Providence, RI;* [4]*Tulane University, New Orleans, LA*

ThP 751 **Single-shot native top-down proteomics on the Corynebacterium diphtheriae exoproteome reveals novel proteoforms, complexes, and functional heme-acquisition system components**; Andrew K Goring[1]; Jordan Ford[1]; Christopher Mullen[2]; Jingjing Huang[2]; Rafael Melani[2]; Robert T. Clubb[1]; Rachel R. Ogorzalek Loo[1]; Joseph A. Loo[1]; [1]*University of California, Los Angeles, Los Angeles, CA;* [2]*ThermoFisher Scientific, San Jose, CA*

ThP 752 **Protein-centric analysis of personalized antibody repertoires – LC-MS-based Fab-profiling on a timsTOF**; Jan Fiala[1,2]; Dina Schuster[1,2]; Simon Ollivier[1,2]; Stuart Pengelley[3]; Markus Lubeck[3]; Florian Busch[4]; Oliver Raether[3]; Jean-François Greisch[4]; Albert J.R. Heck[1,2]; [1]*Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute for Pharmaceutical Sciences, Utrecht University, Padualaan 8, 3584 CH, Utrecht, Netherlands;* [2]*Netherlands Proteomics Center, Padualaan 8, 3584 CH Utrecht, Netherlands;* [3]*Bruker*

Daltonik GmbH & Co. KG, Bremen, Germany; [4]Bruker Daltonik GmbH, Fällanden, Switzerland

ThP 753 **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 754 **An Optimized High-Throughput Top-Down Proteomic Method to Characterize Recombinant RAS Modifications**; Grace M. Scheidemantle[1]; Robert A. D'Ippolito[1]; Matthew R. Drew[1]; Peter Frank[1]; Min Hong[1]; Jennifer Mehalko[1]; Simon Messing[1]; Shelley Perkins[1]; Kelly Snead[1]; Vanessa Wall[1]; Carissa Grose[1]; William Burgan[1]; Dominic Esposito[1]; Frank McCormick[1, 2]; Dwight V. Nissley[1]; Caroline J. DeHart[1]; *[1]Frederick National Laboratory, Frederick, MD; [2]Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA*

ThP 755 **Analysis of intact membrane proteins directly from living bacterial colonies by native LESA mass spectrometry**; Yuying Du[1]; Robin May[1]; Helen Cooper[1]; *[1]University of Birmingham, Birmingham, United Kingdom*

ThP 756 **High Sensitivity Top-down Proteomics for Analysis of Large Proteoforms Enabled by Small-scale Serial Size Exclusion Chromatography**; Holden T Rogers[1]; Jake A Melby[1]; Lauren E Ehlers[1]; Matthew S Fischer[1]; Eli J Larson[1]; Zhan Gao[2]; Kalina J Rossler[2]; Daojing Wang[3]; Andrew J Alpert[4]; Ying Ge[2, 5]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, Wisconsin; [2]University of Wisconsin-Madison, Department of Cell and Regenerative Biology, Madison, WI; [3]Newomics Inc., Berkeley, CA; [4]PolyLC Inc, Columbia, MD; [5]University of Wisconsin-Madison, Department of Chemistry, Madison, WI*

ThP 757 **Exploration of Structural and Relative Stability Information of Protein Complexes by Utilizing D-proline and Native Top-Down MS**; Luchen Wuyang[1]; Boyu Zhao[1]; Rachel Loo[1]; Joseph Loo[1]; *[1]UCLA, Los Angeles, California*

ThP 758 **Site-Selective Cleavage of Proteins by Radical Photoactivation**; Chengwei Chen[1]; Ryan R. Julian[1]; *[1]University of California, Riverside, Riverside, CA*

ThP 759 **A simple and efficient approach for preparing cationic capillary coating for capillary electrophoresis-mass spectrometry-based top-down proteomics**; Qianjie Wang[1, 2]; Guangyao Gao[1]; Peter Lundquist[2]; Liangliang Sun[1]; *[1]Department of Chemistry, Michigan State University, East Lansing, MI; [2]Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI*

ThP 760 **Identification and Verification of Plasma Proteoform Markers from Patients with Progressive Liver Cirrhosis**; Aniel Sanchez[1]; Eleonora Forte[1, 2]; Indira Pla[1]; Che-Fan Huang[1]; Vijaya Lakshmi Kanchustambham[1]; Michael A. Hollas[1]; Troy D Fisher[1]; Katrina N Peterson[1]; Jes M Sanders[2]; Julianna M Doll[2]; Zachary C Dietch[2]; Rafael D Melani[3]; Daniela P Ladner[2]; Michael W Senko[3]; Neil L Kelleher[1, 2]; *[1]Proteomics Center of Excellence, Northwestern University, Evanston, Illinois; [2]Comprehensive Transplant Center, Feinberg School of Medicine, Northwestern University, Chicago, Illinois; [3]Thermo Fisher Scientific, San Jose, CA*

ThP 761 **Evaluating a new Workflow for Top-Down Protein Sequence Confirmation andde novo Sequencing**; Mariangela Kosmopoulou[1]; George Alevizos[1]; Georgia Orfanoudaki[1]; Athanasios Smyrnakis[1]; Michael Greig[2]; Detlev Suckau[3]; *[1]Fasmatech Science and Technology, Athens, Greece; [2]Bruker Scientific, 40 Manning Road, Billerica, MA; [3]Bruker Daltonics, Bremen, Germany*

ThP 762 **Advancing FDR Estimation for Spectral Deconvolution in Top-Down Proteomics**; Ayesha Feroz[1]; Timo Sachsenberg[1, 2]; Konstantin O. Nagornov[3]; Yury O. Tsybin[3]; Oliver Kohlbacher[1, 2, 4]; Kyowon Jeong[1, 2]; *[1]Applied Bioinformatics, Department for Computer Science, University of Tübingen, Sand 14, 72076, Tübingen, Germany; [2]Institute for Bioinformatics and Medical Informatics, University of Tübingen, Sand 14, 72076, Tübingen, Germany; [3]Spectroswiss, 1015, Lausanne, Switzerland; [4]Translational Bioinformatics, University Hospital Tübingen, Hoppe-Seyler-Str. 9, 72076, Tübingen, Germany*

ThP 763 **Novel capillary isoelectric focusing-mass spectrometry techniques for top-down proteomics characterization of histones and nanoparticle protein corona**; Guijie Zhu[1]; Fei Fang[1]; Amirhossein Sadeghi[1]; Liangliang Sun[1]; *[1]Michigan State University, East Lansing, MI*

ThP 764 **FLASHTagger: An open-source web application utilizingde novosequence tags for robust and ion type-free analysis of top-down data**; Kyowon Jeong[1, 2]; Wonhyeuk Jung[3, 4]; Jaywon Lee[3, 4]; Aniruddha Panda[3, 4]; Jared Shaw[5]; Tom D. Müller[1, 2]; Louise M Buur[6]; Viktoria Dorfer[6]; Oliver Kohlbacher[1, 2, 7]; Kallol Gupta[3, 4]; *[1]Applied Bioinformatics, Department for Computer Science, University of Tübingen, Sand 14, 72076, Tübingen, Germany; [2]Institute for Bioinformatics and Medical Informatics, University of Tübingen, Sand 14, 72076, Tübingen, Germany; [3]Yale School of Medicine, New Haven, CT; [4]Nanobiology Institute, Yale University, West Haven, CT; [5]University of Nebraska - Lincoln, Lincoln, NE; [6]University of Applied Sciences Upper Austria, Hagenberg, Austria; [7]Translational Bioinformatics, University Hospital Tübingen, Hoppe-Seyler-Str. 9, 72076, Tübingen, Germany*

ThP 765 **Quantification of age-related proteoform expression changes in cardiac mitochondria using quantitative top-down proteomics**; Kellye A Cupp-Sutton[1]; Anju Teresa Sunny[1]; Andrea Remirez-Sagredo[2]; Ann Chiao[2]; Si Wu[1, 3]; *[1]University of Alabama, Tuscaloosa, AL; [2]Oklahoma Medical Research Foundation, Oklahoma City, Oklahoma; [3]University of Oklahoma, Norman, OK*

ThP 766 **High-precision Proteoform Quantification Reveals Phosphorylation Kinetics of AMP-activated Protein Kinase**; Boris Krichel[1, 2]; Hsin-Ju Chan[1]; Zhan Gao[1]; Charlotte Uetrecht[2, 3]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Siegen, Siegen, Germany; [3]Centre for Structural Systems Biology, Hamburg, Germany*

ThP 767 **Effect of Charge-State Manipulation on Protein Conformation**; Dmitry Eremin[1]; Brandon Nelson[2]; Joshua K McBee[2]; Ashli R Simone[2]; Daniel DeBord[2]; Valery Fokin[1]; *[1]University of Southern California, Los Angeles, CA; [2]MOBILion Systems, Inc., Chadds Ford, PA*

ThP 768 **Enhancing top-down proteomics by novel separation columns coupled to mass spectrometry**; Yu Liang[1]; Yue Sun[1]; Chao Wang[1]; Zhen Liang[1]; Lihua Zhang[1]; Yukui Zhang[1]; *[1]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

ThP 769 **Validating Matching Terminal and Internal Fragments from Targeted Top-Down Proteoform Analyses**; Joseph B. Greer[1, 2]; Bryan P. Early[1, 2]; Daisha Utley[1]; Jessie A. Bolger[1]; Matthew T. Robey[1, 2]; Ryan T. Fellers[1, 2]; Neil L. Kelleher[2]; Kenneth R. Durbin[1, 2]; *[1]Proteinacous, Evanston, IL; [2]Northwestern University, Evanston, IL*

ThP 770 **Characterizing Intact Antibodies Using Ultrafast Sliding Window Deconvolution**; Matthew T. Robey[1]; Daisha Utley[1]; Joseph B. Greer[1, 2]; Ryan T. Fellers[1, 2]; Neil L. Kelleher[1, 2]; Kenneth R. Durbin[1, 2]; *[1]Proteinaceous, Evanston, IL; [2]Northwestern University, Evanston, IL*

ThP 771 **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[1]; Jack L Bennett[1]; Tarick J El-Baba[1]; Di Wu[1]; Joshua D. Hinkle[2]; Christopher Mullen[2]; John E.P. Syka[2]; Idlir Liko[3]; Carol V Robinson[1]; *[1]University of Oxford, Oxford, United Kingdom; [2]ThermoFisher Scientific, San Jose, CA; [3]OMass Therapeutics, Oxford, United Kingdom*

ThP 772 **EXPLORING THE MECHANISM OF MIDDLE DOWN ELECTRON ACTIVATED DISSOCIATION BASED SEQUENCING OF MULTISPECIFIC ANTIBODIES**; Michael

L Poltash[1]; Haichuan Liu[2]; Zoe Zhang[2]; Andrew D Mahan[1]; Hirsh Nanda[1]; *[1]Johnson and Johnson Innovative Medicine, Spring House, Pennsylvania; [2]SCIEX, Redwood City, CA*

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ThP 773 **Quantification of complement membrane attack complex proteins in plasma extracellular vesicles**; Illarion Turko; *Institute for Bioscience and Biotechnology Researc, Rockville, MD*

ThP 774 **Real-time peptide-spectrum rescoring improves sensitivity for sample multiplexed proteomics**; Chris McGann[1]; Erik Bergstrom[1]; Devin Schweppe[1]; *[1]University of Washington, Seattle, WA*

ThP 775 **Establishing a low-input mouse immune cell proteomic atlas with unit-resolution mass spectrometry for targeted library generation**; Ariana E Shannon[1]; Nojoon Soon[1]; Yi Wang[1]; Teeradon Phlairaharn[2]; Lilian R Heil[3]; Cristina Jacob[3]; Philip M. Remes[3]; Brian Searle[1]; *[1]The Ohio State University, Columbus, OH; [2]Thermo Fisher Scientific, Bremen, Germany; [3]Thermo Fisher Scientific, San Jose, CA*

ThP 776 **Quantifying the metabolic proteome**; Yassene Mohammed[1, 2, 3]; Vincent R. Richard[1]; Claudia Gaither[4]; Robert Popp[4]; Christoph H. Borchers[1, 3, 5, 6]; *[1]Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC; [2]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [3]Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC; [4]MRM Proteomics Inc, Montreal, QC; [5]Division of Experimental Medicine, McGill University, Montreal, QC; [6]Department of Pathology, McGill University, Montreal, QC*

ThP 777 **Deep, unbiased and quantitative mass spectrometry-based plasma proteome analyses of personalized response to mRNA COVID-19 vaccine**; Ting Huang[1]; Alex Rosa Campos[2]; Jian Wang[1]; Alexey Stukalov[1]; Ramón Díaz[3]; Svetlana Maurya[3]; Khatereh Motamedchaboki[1]; Daniel Hornburg[1]; Laura R. S. Oliveira[4]; Camila I. Alves[4]; Rafael L. Rosa[4]; Yohana P. Calegari-Alves[4]; Serafim Batzoglou[1]; Lucélia Santi[4]; Walter O. Beys-da-Silva[4]; *[1]Seer, Inc., Redwood City, CA; [2]Plexium, San Diego, CA; [3]Sanford Burnham Prebys, San Diego, California; [4]Federal University of Rio Grande do Sul, Porto Alegre, Brazil*

ThP 778 **Providing an analytical platform for state-of-the-art absolute apolipoprotein quantification in human blood plasma using prm-PASEF**; David Kotol[1]; Christian Albers[2]; Stephanie Kaspar-Schoenefeld[2]; *[1]ProteomEdge, Stockholm, Sweden; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

ThP 779 **Exploring Human Serum Proteome Profiles in Response to Chronic and Acute Exposure to Organophosphate Pesticides using LC-MS/MS**; Mojgan Atashi[1]; Dina El-Gameel[2]; Vishal Sandilya[1]; Thu Nguyen[1]; Md Mostofa Al Amin Bhuiyan[1]; Judith Ijeoma Nwaiwu[1]; Noha A. Hamdy[3]; Maha A. Ghanem[4]; Labiba K El-Khordaugi[3]; Salwa M. Abdallah[5]; Ahmed El-Yazbi[6]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas; [2]Alexandria University Hospitals, Alexandria, Egypt; [3]Faculty of Pharmacy, Alexandria University, Egypt, Alexandria, Egypt; [4]Faculty of Medicine, Alexandria University, Alexandria, Egypt; [5]Central Agricultural Pesticides Lab (CAPL), Agricultural Research Center (ARC), Cairo, Egypt, Cairo, Egypt; [6]Department of Pharmacology and Therapeutics, Faculty of Pharmacy, Alamein International University, Alamein, Egypt*

ThP 780 **Amyotrophic Lateral Sclerosis-Associated Mutants of SOD1 Altered mRNA Splicing through Their Aberrant Interactions with SRSF2**; Xingyuan Chen[1]; Zhongwen Cao[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

ThP 781 **Real-Time Search enables sensitive and accurate TMTproC quantification of transcription factors during embryogenesis**; Alex Johnson[1]; Jingjing Huang[2]; Argit Marishta[1]; Edward Cruz[1]; Andrea Mariossi[1]; William Barshop[2]; Jesse D. Canterbury[2]; Rafael Melani[2]; David Bergen[2]; Vlad Zabrouskov[2]; Graeme McAlister[2]; Martin Wühr[1]; *[1]Princeton University, Princeton, NJ; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 782 **Multi-modal proteome atlas to enhance treatment capability of KRAS-driven cancers**; Syed Azmal Ali[1]; Karim Aljakouch[1]; Jeroen Krijgsveld[1, 2]; *[1]German Cancer Research Center, Heidelberg, Germany; [2]Heidelberg University, Medical Faculty, Heidelberg, Germany*

ThP 783 **Characterization of aging-related adaptive naïve and innate immune human proteomes**; Ceereena Ubaida-Mohien[1]; Alexey Lyashkov[1]; Amit Singh[1]; Mary Kaileh[1]; Arsun Bektas[1]; Yevgeniya Lukyanenko[1]; Jaekwan Kim[1]; Julián Candia[1]; Nan Ping Weng[1]; Ranjan Sen[1]; Luigi Ferrucci[1]; *[1]National Institute on Aging, National Institutes of Health, Baltimore, MD 21224*

ThP 784 **Metabolic labeling to describe extracellular matrix proteome dynamics in a fibrin-based in vitro wound healing model**; Dalton Miles[1]; Kathryn Jacobson[2]; Adrian Buganza-Tepole[3]; Sarah Calve[1]; *[1]University of Colorado Boulder, Boulder, CO; [2]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA; [3]Purdue University, West Lafayette, IN*

ThP 785 **Optimization of narrow isolation windows with Zeno SWATH-DIA for improving proteomic identification**; Kongxin Gu[1]; Haruka Kumabe[1]; Takumi Yamamoto[1]; Naoto Tashiro[1]; Takashi Masuda[2]; Shingo Ito[1]; Sumio Ohtsuki[1]; *[1]Kumamoto University, Kumamoto, Japan; [2]Keio University, Tsuruoka, Japan*

ThP 786 **Targeted proteomics reveals the regulation of the Polycomb Repressive Complex 1 by USP7 and its involvement in neurodevelopment**; Joyce Wolf Van Der Meer[1]; Ayestha Sijm[1]; Axelle Larue[2]; Yaser Atlasi[2]; Jan A Van Der Knaap[1]; Gillan E Chalkley[1]; Karel Bezstarosti[1]; Dick HW Dekkers[1]; Wouter AS Doff[1]; Zeliha Ozgur[1]; Wilfred FJ Van Ijcken[1]; Peter C Verrijzer[1]; Jeroen AA Demmers[1]; *[1]Erasmus University Medical Center, Rotterdam, Netherlands; [2]Queen's University Belfast, Belfast, United Kingdom*

ThP 787 **Global proteomics and integrative thermal proteome profiling of hepatic stellate cells in liver fibrogenesis**; Ian Green[1]; James Rooney[1]; Chunna Guo[1]; Whitney Smith-Kinnaman[1]; Jessica Maiers[1]; Amber L Mosley[1]; *[1]Indiana University School of Medicine, Indianapolis, IN*

ThP 788 **Accurate multiplexed proteomics on a quadrupole-ion trap instrument**; Edward R Cruz[1]; Alex Johnson[1]; Thao Nguyen[1]; Jessica Wang[1]; Michael Stadlmeier[1]; Philip M Remes[2]; Graeme McAlister[2]; Martin Wuhr[1]; *[1]Princeton University, Princeton, NJ; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 789 **Bayesian Confidence Intervals for Absolute Protein Quantification**; Vyas Pujari[1, 2]; Chirag Kumar[1, 2]; Meera Gupta[1, 2]; Donovan Cassidy-Nolan[1, 2]; Arjuna Subramanian[1, 2]; Martin Wühr[1, 2]; *[1]Princeton University, Princeton, NJ; [2]Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ*

ThP 790 **The Association of Biomolecular Resource Facilities Proteomics Standards Research Group (sPRG) Multi-Species Standard to Assist Quantitative Proteomics**; Benjamin A. Neely[1]; Josue Baeza[2]; Magnus Palmblad[3]; Lindsay K Pino[4]; Brian C Searle[5]; Susan T. Weintraub[6]; *[1]National Institute of Standards and Technology, Charleston, SC; [2]GSK, Collegeville, PA; [3]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [4]Talus Bioscience, Seattle, WA; [5]Department of Biomedical Informatics, The Ohio State University Medical Center, Columbus, OH; [6]Univ. of Texas HSC, San Antonio, TX*

ThP 791 **A cross-species Proteomic assessment of cost-effective platforms for depleting high-abundant proteins from blood serum**; Zongkai Peng[1]; Shakya Sankalpani Gunasena Wije Munige[1]; Deepti Bhusal[1]; Isabella Yang[2]; Zhibo Yang[1]; Nagib Ahsan[1, 3]; *[1]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK; [2]Norman North Highschool, Norman, OK; [3]Mass*

Spectrometry, Proteomics and Metabolomics Core Facility, Stephenson Life Sciences Research Center, The University of Oklahoma, Norman, OK

ThP 792 **Democratizing Plasma Proteomics: Massively Parallel Targeted Analysis Using a Novel Hybrid Nominal Mass Resolution Tandem Mass Spectrometer**; Christine C. Wu[1]; Philip M. Remes[2]; Cristina C. Jacob[2]; Deanna Plubell[1]; Lilian R Heil[2]; Bo Wen[1]; Nicholas Shulman[1]; Brendan MacLean[1]; Michael MacCoss[1]; *[1]University of Washington, Seattle, WA; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 793 **TranslationofProteograph XT Nanoparticle-Enriched Plasma proteomic features to a targeted assay**; Yi (JIMMY) Zeng[1]; Philip M Remes[2]; Cristina C. Jacob[2]; Hao Qian[1]; Megan Mora[1]; Sangeet Adhikari[1]; Isabella Bonomi[1]; Purva Ranjan[1]; Alan Atkins[2]; Scott M Peterman[2]; Claudia Martins[2]; Philip Ma[1]; Bruce Wilcox[1]; *[1]PrognomiQ Inc, San Mateo, CA; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 794 **Unraveling Molecular Details Underlying COP9 Signalosome-mediated Regulation of Cullin-RING Ligases Using Quantitative Cross-linking Mass Spectrometry**; Xiaorong Wang[1]; Clinton Yu[2]; Fenglong Jiao[2]; Haibin Mao[3]; Ning Zheng[3]; Lan Huang[2]; *[1]University of California-Irvine, IRVINE, CA; [2]University of California Irvine, Irvine, CA; [3]University of Washington, Seattle, WA*

ThP 795 **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[1, 2]; Vena Martinez[1]; Weiwei Wang[1, 2]; Florine Collins[1, 2]; TuKiet T. Lam[1, 2]; Matthew Girgenti[1]; *[1]Yale School of Medicine, New Haven, CT; [2]Keck MS & Proteomics Resource, New Haven, CT*

ThP 796 **Proteomic evaluation of tardigrades following ionizing radiation reveals increase in DNA repair pathways**; Evan R Stair[1]; Courtney Clark-Hatchel[1, 2]; Bob Goldstein[1]; Leslie M. Hicks[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]University of North Carolina at Asheville, Asheville, NC*

ThP 797 **Absolute quantification of photoreceptor outer segment proteins**; Nikolai Skiba[1]; Tylor R. Lewis[1]; William J. Spencer[2]; Carson M. Castillo[1]; Andrej Shevchenko[3]; Vadim Y. Arshavsky[1]; *[1]Duke University, Durham, NC; [2]SUNY Upstate Medical University, Syracuse, NY; [3]Max Plank Institute of Molecular Cell Biology and Geretics, Dresden, Germany*

ThP 798 **Evaluating different recombinant Trypsin sequences for enhanced MS-based peptide identification and quantitative analysis**; Cristina Hernandez Rollan[1]; Tanveer Singh Batth[1]; Morten H. H. Nørholm[2]; Jesper Velgaard Olsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, Copenhagen, Denmark; [2]Novo Nordisk Foundation Center for Biosustainability, Denmark Technical University, Lyngby, Denmark*

ThP 799 **High-throughput LC-MS/MS enables protein Quantitative Trait Loci mapping in the progression of Metabolic Dysfunction-Associated Steatotic Liver Disease**; Margaret Lea Robinson[1]; Giorgia Benegiamo[2]; Jean-David Morel[2]; Wenyu Liu[2]; Katherine A Overmyer[1, 3, 4]; Johan Auwerx[2]; Joshua J Coon[1, 3, 4, 5]; *[1]University of Wisconsin-Madison, Department of Biomolecular Chemistry, Madison, WI; [2]Laboratory of Integrative Systems Physiology, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; [3]Morgridge Institute for Research, Madison, WI; [4]National Center for Quantitative Biology of Complex Systems, Madison, WI; [5]University of Wisconsin-Madison, Department of Chemistry, Madison, WI*

ThP 800 **Extended Characterization and Multiplexed Quantification via a Chemical Proteomics Platform Using High-field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS)**; Hung-Yu (Eric) Chiang[1, 2]; Min Ma[1]; Miyang Li[3]; Lingjun Li[1, 3]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Biophysics Program, University of Wisconsin-Madison, Madison, Wisconsin; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

ThP 801 **Characterization of Proteins in Pig Sertoli Cells to Understand Complement System Behavior and Possible Xenotransplantation Applications Using LC-MS/MS Techniques**; Andrew I. Bennett[1]; Rachel Washburn[2]; Moyinoluwa Adeniyi[1]; Vishal Sandilya[1]; Jannette M. Dufour[3]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Ivy Tech Community College, Department of Life and Physical Sciences, Sellersburg, IN; [3]Texas Tech University Health Sciences Center, Lubbock, TX*

ThP 802 **Unleashing the Power of HT-DIA Acquisition on Orbitrap Exploris 240 – Precise and Accurate Quantitation at 260 SPD**; Maciej Bromirski[1]; Dominic Hoch[2]; Julia Kraegenbring[3]; Riccardo Stucchi[2]; Jeff Op De Beeck[4]; Robert Van Ling[4]; *[1]Thermo Fisher Scientific, Warsaw, Poland; [2]Thermo Fisher Scientific GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, Bremen, Germany; [4]Thermo Fisher Scientific, Ghent, Belgium*

ThP 803 **Innovative approaches for an in- depth quantitative analysis of the serum proteome of brown bears**; Alexandre GEFFROY[1]; Hugo GIZARDIN-FREDON[1]; Jon ARNEMO[2]; Jonas KINDBERG[3]; Sarah CIANFERANI[1]; Guillemette GAUQUELIN-KOCH[4]; Lydie COMBARET[5]; Etienne LEFAI[5]; Fabrice BERTILE[1]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, IPHC, UMR 7178, ProFI FR2048, CNRS Université de Strasbourg, Strasbourg, France; [2]Inland Norway University of Applied Sciences, Koppang, Norway; [3]Norwegian Institute for Nature Research, Trondheim, Norway; [4]Centre National d'Etudes Spatiales, Paris, France; [5]Université Clermont Auvergne, INRAE, UNH UMR 1019, Clermont-Ferrand, France*

ThP 804 **Novel Hybrid Nominal Mass Instrument Enables Rapid Development of Large-Scale Targeted Plasma Proteomics Assays**; Yi (JIMMY) Zeng[1]; Philip M Remes[2]; Sangeet Adhikari[1]; Cristina C. Jacob[2]; Hao Qian[1]; Megan Mora[1]; Isabella Bonomi[1]; Purva Ranjan[1]; Alan Atkins[2]; Claudia Martins[2]; Philip Ma[1]; Bruce Wilcox[1]; *[1]PrognomiQ Inc, San Mateo, CA; [2]Thermo Fisher Scientific, San Jose, CA*

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ThP 805 **Cold skeletal muscle slices: A new approach to spatial visualisation of protein profiles**; Luisa Schmidt[1, 2]; Marcus Krüger[1, 2]; Philipp Antczak[2, 3]; Abigail Mackey[4, 5]; Christian Hoegsbjerg[4, 5]; Michael Saynisch[2]; *[1]University of Cologne, Cologne, Germany; [2]CECAD (Cluster of Excellence in Cellular Stress Responses in Aging-Associated Diseases), Cologne, Germany; [3]CMMC (Center for Molecular Medicine), Cologne, Germany; [4]Institute of Sports Medicine Copenhagen, Copenhagen, Denmark; [5]University of Copenhagen, Copenhagen, Denmark*

ThP 806 **Shared peptides among diverse lineages of marine microeukaryotes**; Natalie Cohen[1]; Jaclyn K Saunders[2]; Mak A Saito[3]; *[1]University of Georgia, Savannah, GA; [2]University of Georgia, Athens, GA; [3]Woods Hole Oceanographic Institution, Falmouth, MA*

ThP 807 **Illuminating the human phosphoproteome through the lens of clinical kinase inhibitors**; Florian P Bayer[1]; Julian Müller[1]; Matthew The[1]; Bernhard Kuster[1, 2]; *[1]Technical University of Munich, Freising, Germany; [2]German Cancer Consortium (DKTK), Partner Site Munich, Munich, Germany*

ThP 808 **Data-Driven Modeling of the Mouse Macrophage Toll-like Receptor Signaling Pathway**; Nathan P Manes[1]; Sergio A Hassan[1]; Anthony A Armstrong[1]; Fengkai Zhang[1]; Rachel A Gottschalk[2]; Matthew J Marino[1]; Iain DC Fraser[1]; Ronald N Germain[1]; Martin Meier-Schellersheim[1]; Aleksandra Nita-Lazar[1]; *[1]National Institutes of Health, Bethesda, MD; [2]University of Pittsburgh, Pittsburgh, PA*

ThP 809 **Metabolite-protein architecture in the diversity outbred population defines mechanisms of control over metabolic pathways**; Haopeng Xiao[1]; Martha Ordonez[1]; Nils Burger[1]; Shelley M Wei[2]; Sumeet Khetarpal[1, 3]; Edward L. Huttlin[4]; Edward T Chouchani[1]; *[1]Dana-Farber*

Cancer Institute/ Harvard Medical School, Boston, MA; [2]Dana-Farber Cancer Institute, Boston, MA; [3]MGH, boston, MA; [4]Harvard Medical School, Boston, MA

ThP 810 **Tumor ecosystem Interrogating via an multiomics strategy identifies novel therapeutic vulnerabilities for drug-resistant Acute Myeloid Leukemia patients**; Long Shen[1]; Yang Yang[1]; Chunliang Li[2]; Hong Wang[1]; *[1]State key laboratory of blood science, Institute of Hematology & Blood Diseases Hospital, Chinese Academy of Medical Sciences & Peking Union Medical College, Tianjin, China; [2]St Jude Children's Research Hospital, Memphis, TN*

ThP 811 **High Throughput Simultaneous Multi-Omics Analysis by Direct Infusion Mass Spectrometry (SMAD-MS)**; Yuming Jiang[1]; Ivan Salladay-Perez[2]; Amanda Momenzadeh[1]; Anthony J Covarrubias[2]; Jesse Meyer[1]; *[1]Cedars-Sinai Medical Center, Los Angeles, CA; [2]University of California, Los Angeles, Los Angeles, CA*

ThP 812 **Synchrotron Radiolysis as Synthetic Reactive Oxygen Species Source Drives Methionine Sulfoxide Accumulation in ROS Sensitive E. coliProteins.**; Ezaz Ahmed[1, 2]; Erik R. Farquhar[1, 2]; Daniela Schlatzer[3]; Janna Kiselar[2, 4]; David T. Lodowski[2, 4]; Mark R. Chance[1, 2, 4]; *[1]Center for Synchrotron Biosciences, Case Western Reserve University, School of Medicine, Cleveland, OH; [2]Department of Nutrition, Case Western Reserve University, School of Medicine, Cleveland, OH; [3]Center for Proteomics and Bioinformatics, Department of Nutrition, Case Western Reserve University, Cleveland, OH; [4]Center for Proteomics and Bioinformatics, Case Western Reserve University, School of Medicine, Cleveland, OH*

ThP 813 **Deciphering age-dependent global proteome changes in the leaf-cutting antAcromyrmex echinatiorfor better understanding of biomineralization process**; Penghsuan Huang[1]; Joseph Sardina[2]; Haiyan Lu[3]; Cameron R. Currie[2]; Lingjun Li[3]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Department of Bacteriology, University of Wisconsin-Madison, Madison, WI; [3]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

ThP 814 **The proteomic landscape of interferon signaling in primary human T cells and lung cells**; Christian M. Beusch[1]; Christopher Monaco[1]; David Ezra Gordon[2]; Samuel Gallant[1]; *[1]Emory University School of Medicine, Atlanta, GA; [2]Emory University, Atlanta, GA*

ThP 815 **Formaldehyde crosslinking coupled RNA interactome capture at peptide-level enabled robust profiling of RNA-binding regions**; Seonmin Ju[1, 2]; Yongwoo Na[1, 2]; Jong-Seo Kim[1, 2]; *[1]School of Biological Sciences, Seoul National University, Seoul, South Korea; [2]Center for RNA Research, Institute of Basic Science (IBS), Seoul, South Korea*

ThP 816 **Global affinity-based organelle profiling reveals subcellular localization and remodeling at proteome scales**; Duo Peng[1]; Marco Y Hein[1, 2]; Verina Todorova[1]; Frank McCarthy[1]; Kibeom Kim[1]; Chad Liu[1]; Laura Savy[1]; Camille Januel[3]; Rodrigo Baltazar-Nunez[3]; Sophie Bax[1]; Brian C DeFelice[1]; Shalin B Mehta[1]; Daniel N Itzhak[3, 4]; Manuel D Leonetti[1]; Joshua E Elias[1]; *[1]Chan-Zuckerburg Biohub, San Francisco, California; [2]Max Perutz Laboratories Vienna, Vienna BioCenter, Vienna, Austria; [3]Chan Zuckerberg Biohub, San Francisco, CA; [4]Altos Labs, Redwood City, California*

ThP 817 **Quantification of cell-type specific protein dynamics in Drosophila embryos**; Argit Marishta[1]; Martin Wühr[1]; Eric Wieschaus[1]; *[1]Princeton University, Princeton, NJ*

ThP 818 **A subcellular proteome map of a marine organism using the Orbitrap Astral mass spectrometer**; Loay J. Jabre[1]; Matthew R. McIlvin[1]; Mak A. Saito[1]; *[1]Woods Hole Oceanographic Inst., Woods Hole, MA*

ThP 819 **Evidence for widespread mesoscale cytoplasmic organization into condensates by quantitative proteomics of cell extract filtrates**; Felix C Keber[1]; Thao Nguyen[1]; Andrea Mariossi[1]; Clifford P Brangwynne[1, 2]; Martin Wühr[1]; *[1]Princeton University, Princeton, NJ; [2]Howard Hughes Medical Institute, Chevy Chase, MD*

ThP 820 **Deciphering hierarchical cell cycle controls with phosphoproteomics**; Anthony Cesnik[1, 2, 3]; Christian Gnann[2, 4]; Frank McCarthy[3]; Daniel Itzhak[3]; Emma Lundberg[1, 2, 3]; *[1]Stanford University, Stanford, CA; [2]KTH Royal Institute of Techonology, Stockholm, Sweden; [3]Chan Zuckerberg Biohub, San Francisco, CA; [4]Chan-Zuckerburg Biohub, San Francisco, CA*