



71st CONFERENCE

Mass Spectrometry
and Allied Topics

June 4 - 8, 2023



SHORT COURSES
June 3 & 4



FINAL PROGRAM

The detailed final program book is no longer printed and distributed at the conference. This file represents the conference program as of April 23, 2023.

Late-breaking program changes and alerts are available through the online planner and mobile app.

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SATURDAY, JUNE 3, 2023

9:00 AM - 5:00 PM	SHORT COURSES (Badge printing for short courses is 8-9am)
2:00 - 5:00 PM	NAME BADGE PRINTING & INFORMATION , Level One Lobby (outside Hall B)

SUNDAY, JUNE 4, 2023

9:00 AM - 5:00 PM	SHORT COURSES (Badge printing for short courses is 8-9am)	
10:00 AM - 8:00 PM	NAME BADGE PRINTING & INFORMATION , Level One Lobby (outside Hall B)	
4:00 - 4:45 PM	ATTENTION: FIRST-TIME GRADUATE STUDENTS AND UNDERGRADUATE STUDENTS Plan your Strategy: What to See and Do at ASMS , Hall B3	
5:00 - 5:45 PM	TUTORIAL SESSION I , Hall B3 5:00 – 5:45 pm Mass Spectrometry and Medicine Livia Eberlin <i>Baylor College of Medicine</i>	TUTORIAL SESSION II , Ballroom A 5:00 – 5:45 pm Mass Spectrometry and Anti-Doping Research Mario Thevis <i>Institute of Biochemistry, Center for Preventive Doping Research, German Sport University Cologne</i>
	SPECIAL KEYNOTE SESSION , Hall B3 Activism in Houston - Boots on the Ground: Progress & Challenges Jeremy Edwards , Chair, Houston LGBTQ Advisory Board	
6:45 - 7:45 PM	CONFERENCE OPENING PLENARY , Hall A Welcome, Joseph A. Loo , <i>University of California, Los Angeles</i> ASMS Vice President for Programs 7:00 - 7:45 pm You are what you eat - the study of post-prandial protein handling in vivo in humans Luc J.C. van Loon <i>Department of Human Biology at Maastricht University Medical Centre+</i>	
7:45 - 9:00 PM	WELCOME RECEPTION , Posters-Exhibits Hall (Level One) Join us to celebrate the conference opening, visit exhibit booths. The Undergraduate Student Poster Competition is conducted during the reception. Competition posters are displayed beginning on poster board 001.	

MONDAY, JUNE 5, 2023

7:00 AM	CORPORATE BREAKFAST SEMINARS , Convention Center (Level Three) and Hilton Americas
7:30 AM - 5:00 PM	NAME BADGE PRINTING & INFORMATION , Level One Lobby (outside Hall B)
8:30 - 10:30 AM	<p>ORAL SESSIONS</p> <p>MOA am: Top Down Protein Analysis, Hall B3 MOB am: Imaging: Instrumentation & Method Development, Grand Ballroom A MOC am: Clinical Analysis: Innovations, Grand Ballroom B MOD am: Small Molecules: Structural Characterization and Quantitation, Grand Ballroom C MOE am: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements, Room 332 MOF am: Covalent Labeling and Chemical Crosslinking, General Assembly A MOG am: Polymers, General Assembly B MOH am: Informatics: Metabolomics and Lipidomics, General Assembly C</p>
10:30 AM - 2:30 PM	<p>POSTER SESSION AND EXHIBITS, Monday Posters, Halls BC</p> <p>Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm</p> <p>11:30 am - 1:00 pm: Undergraduate students look for reserved tables and free lunch vouchers to <i>Meet the Experts</i></p>
2:30 - 4:30 PM	<p>ORAL SESSIONS</p> <p>MOA pm: Single Cell Omics, Hall B3 MOB pm: Ion Mobility: Instrumentation & Method Development, Grand Ballroom A MOC pm: Structural Biology, Grand Ballroom B MOD pm: Data-Independent Acquisition and Multiplexing: Lipidomics and Metabolomics, Grand Ballroom C MOE pm: Food Safety & Chemistry: Innovations, Room 332 MOF pm: Cancer Research, General Assembly A MOG pm: Fundamentals: Unconventional Approaches in MS, General Assembly B MOH pm: High Throughput MS, General Assembly C</p>
4:45 - 5:30 PM	<p>AWARD LECTURE, Hall A</p> <p>John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry preceded by Al Yergey MS Scientist Award Presentations</p> <p>Carol V. Robinson <i>University of Oxford</i></p>
5:45 - 7:00 PM	<p>WORKSHOPS There are light refreshments in foyers, 5:30 - 5:45 pm.</p> <p>01 The Role of Mass Spectrometry in Emerging Energy Technologies Development, Room 310 A 02 Nucleic Acids Mass Spectrometry: Emerging Applications, Effective Analytical Strategies, and Characterization for Progressively Larger Nucleic Acids, Room 310 BC 03 Research and Funding Opportunities at the FDA: Mass Spectrometry for Drug Product Quality, Room 320 A 04 Global participatory efforts to characterize the biochemical composition of food: The Periodic Table of Food Initiative and The Proteomes that Feed the World, Room 320 AB 05 Single-Cell Proteomic Standardization: From Study Design to Data Analysis, Ballroom A 06 Networking for Scientists: Celebrating Women Mass Spectrometrists, Ballroom B 07 Exploring the World of Mass Spectral Libraries, Library Search Software and Their Applications , Ballroom C 08 Ion traps as reaction vessels, Room 332 09 Career Opportunities for Chinese Students and Scholars, General Assembly A 10 Making Top-Down Mass Spectrometry Easier to Develop and Apply: Ways to Work Together and How Everyone Can Contribute, General Assembly B 11 New Aspects in the Development and Implementation of Multi-Attribute Method (MAM), General Assembly C 12 Data quality in the core lab: Preventing, catching, reporting and sometimes even fixing! suboptimal "bad data" in a omics core facility aka the "Bad data Workshop", Room 340 AB 13 Emerging Techniques for Rapid Fabrication in MS Laboratories, Room 351 ABDE 14 Cannabis & Hemp Science: The Importance of Mass Spectrometry, Room 351 CF 15 Mind the (Translation) Gap , Room 360 ABDE 16 Exosome research: overcoming challenges to deliver answers, Room 360 CF 17 Using Casanovo for de novo peptide sequencing, Room 361 ABDE</p>
7:00 - 8:00 PM	<p>SPECIAL GAP HOUR RECEPTION SPONSORED BY AGILENT, Ballroom B</p> <p>Reception immediately following workshop <i>06 Networking for Scientists: Celebrating Women Mass Spectrometrists</i>. All are welcome to join for networking focused on supporting women in mass spectrometry and the FeMS organization.</p>
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES AT HILTON AMERICAS

TUESDAY, JUNE 6, 2023

7:00 AM	CORPORATE BREAKFAST SEMINARS , Convention Center (Level Three) and Hilton Americas
7:30 AM - 5:00 PM	NAME BADGE PRINTING & INFORMATION , Level One Lobby (outside Hall B)
8:30 - 10:30 AM	<p>ORAL SESSIONS</p> <p>TOA am: Instrumentation: New Developments in Ionization and Sampling (In Memory of Marvin Vestal), Hall B3</p> <p>TOB am: Biomarkers: Quantitative Analysis, Grand Ballroom A</p> <p>TOC am: Fundamentals: Native MS and Structures of Large Ions , Grand Ballroom B</p> <p>TOD am: Informatics: Peptide and Protein Identification, Proteomics, Grand Ballroom C</p> <p>TOE am: Exposomics, Toxicology, and Health Outcomes, Room 332</p> <p>TOF am: Neurodegenerative Disease Research, General Assembly A</p> <p>TOG am: Drug Metabolism and Pharmacokinetics, General Assembly B</p> <p>TOH am: Imaging: Spatially-Resolved Omics, General Assembly C</p>
10:30 AM - 2:30 PM	<p>POSTER SESSION AND EXHIBITS, Tuesday Posters, Halls BC</p> <p>Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm</p> <p>Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm</p>
2:30 - 4:30 PM	<p>ORAL SESSIONS</p> <p>TOA pm: Instrumentation: High-Resolution Mass Spectrometry, Hall B3</p> <p>TOB pm: Post-translational Modifications: Qualitative & Quantitative Analysis, Grand Ballroom A</p> <p>TOC pm: Fundamentals: Ionization Methods, Grand Ballroom B</p> <p>TOD pm: Informatics: Multiomics Integration and Applications, Grand Ballroom C</p> <p>TOE pm: Plants and Natural Products, Room 332</p> <p>TOF pm: Ion Mobility: Structure Determination & Applications, General Assembly A</p> <p>TOG pm: H/D Exchange: Innovations and Applications, General Assembly B</p> <p>TOH pm: Clinical Analysis: Applications, General Assembly C</p>
4:45 - 5:30 PM	<p>AWARD LECTURE, HALL B3</p> <p>Biemann Medal Lecture preceded by Research Award Presentations</p> <p>Brandon Ruotolo <i>University of Michigan</i></p>
5:45 - 7:00 PM	<p>WORKSHOPS There are light refreshments in foyers, 5:30 - 5:45 pm.</p> <p>01 Open and Reproducible Data Analysis for FT-MS, Room 310 A</p> <p>02 Accelerator Mass Spectrometry (AMS): Current Utility and Future Opportunities , Room 310 BC</p> <p>03 Constructing an Individual Development Plan (IDP), Room 320 A</p> <p>04 The NIH and NSF Review and Funding Process, Room 320 BC</p> <p>05 From data to biology: using -omics datasets to generate an unbiased hypothesis , Ballroom A</p> <p>06 Recognizing the “A” in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists, Ballroom B</p> <p>07 Data Independent Acquisition: After the Acquisition, Ballroom C</p> <p>08 FAIR Data Sharing Principles and Barriers: the New NIH Data Management and Sharing (DMS) Policy, Room 332</p> <p>09 Kahoot Trivia! LCMS (and other topics) , General Assembly A</p> <p>10 Lipidomics: What does International Lipidomics Society offer to the lipidomic community?, General Assembly B</p> <p>11 Native MS: new approaches to enable discovery in academia and industry, General Assembly C</p> <p>12 New fragmentation methods as seen through the lens of radical ion chemistry, Room 340 AB</p> <p>13 Non-target analysis (NTA): Modern tools for unknown analysis, Room 351 ABDE</p> <p>14 Trans-Proteomic Pipeline: Recent Advances and Future Directions, Room 351 CF</p> <p>15 Imaging MS: Isomer Differentiation in Biological Imaging, Room 360 ABDE</p> <p>16 Mass Spectrometry Support for Extractables and Leachables and Biocompatibility testing, Room 360 CF</p> <p>17 Mass Spectral Tools to Enhance Characterization and Identification of Forensic Evidence, Room 361 ABDE</p> <p>17 Visualization of Mass Spectrometry related data (Interest Group: Bioinformatics MS), Room 200 HI</p>
7:00 - 8:00 PM	<p>SPECIAL GAP HOUR RECEPTION SPONSORED BY SCIEX, Ballroom B</p> <p>Reception immediately following workshop <i>06 Recognizing the “A” in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists</i>. All are welcome to join for networking focused on accessibility, diversity and inclusion.</p>
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES AT HILTON AMERICAS

WEDNESDAY, JUNE 7, 2023

7:00 AM	CORPORATE BREAKFAST SEMINARS , Convention Center and Hilton Americas
7:30 AM - 5:00 PM	NAME BADGE PRINTING & INFORMATION , Level One Lobby (outside Hall B)
8:30 - 10:30 AM	<p>ORAL SESSIONS</p> <p>WOA am: Instrumentation: New Hybrid and Multimodal Approaches, Hall B3 WOB am: Biotherapeutics: Characterization and Quantitation, Grand Ballroom A WOC am: Drug Discovery and Development: Qualitative and Quantitative Analysis, Grand Ballroom B WOD am: Artificial Intelligence in MS Instrumentation and Applications, Grand Ballroom C WOE am: Industry: Trace Analysis, Quality Control, and Automation, Room 332 WOF am: Lipidomics: New MS Technologies and Applications, General Assembly A WOG am: Stable Isotope Labeling: Applications, General Assembly B WOH am: Fundamentals: Ion Activation and Dissociation (Honoring Jean Futrell), General Assembly C</p>
10:30 AM - 2:30 PM	<p>POSTER SESSION AND EXHIBITS, Wednesday Posters, Halls BC</p> <p>Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm</p>
2:30 - 4:30 PM	<p>ORAL SESSIONS</p> <p>WOA pm: Instrumentation: Detection of High-Mass Analytes, Hall B3 WOB pm: Biomarkers: Qualitative Analysis , Grand Ballroom A WOC pm: Metabolomics: New Technologies and Applications, Grand Ballroom B WOD pm: Challenges in MS Analysis of Complex Mixtures, Grand Ballroom C WOE pm: GC/MS: Instrumentation and Applications, Room 332 WOF pm: Quantitative Proteomics in Systems Biology, General Assembly A WOG pm: Fundamentals: Reactions of Gaseous and Solvated Ions, General Assembly B WOH pm: Environmental: Non-Target Analysis and Emerging Contaminants, General Assembly C</p>
4:45 - 5:30 PM	ASMS MEETING , Hall B3. Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 PM	<p>WORKSHOPS There are light refreshments in foyers, 5:30 - 5:45 pm.</p> <p>01 High throughput screening mass spectrometry - current status and future landscape, Room 310 A 02 Late-Night Lightning Lectures! , Room 310 BC 03 Utilizing GC/MS Technologies and Associated Software Tools to Address Challenging Applications in the Flavor, Fragrance and Foodstuffs Laboratory , Room 320 A 04 Biomarkers Development: How Mass Spectrometry Is Changing the Field, Room 320 BC 05 Ion Mobility Spectrometry: From Data to Structure, Ballroom A 06 MS Career Options: How to Kick Start Your Career, Ballroom B 07 Ambient Ionization in Application Fields: What is Required, Desired, and Provided?, Ballroom C 08 Target Protein Degradation and MS-based Proteomics , Room 332 09 What are the future needs of photoionization mass spectrometry for complex mixture analysis?, General Assembly A 10 Houston, We Have a Microbiome Problem (...and how the Metaproteomics Initiative aims to solve it!), General Assembly B 11 Hispanics and Latinx in Mass Spectrometry, General Assembly C 12 Polymeric materials: tackling hydrocarbon-based polymers, Room 340 AB 13 ProteomicsML: An online educational platform for machine learning in proteomics, Room 351 ABDE 14 Art, Museums, and Archaeology, Room 351 CF 15 Remote Sample Collection and Microsampling is Driving New Mass Spectrometry Analytical Solutions, Room 360 ABDE 16 Knowledge Share and Instrumentation Donations for Developing World Outreach, Room 360 CF</p>
7:00 - 8:00 PM	<p>SPECIAL GAP HOUR RECEPTION SPONSORED BY SEER, Ballroom B</p> <p>Reception immediately following workshop <i>06 MS Career Options: How to Kick Start Your Career</i>. All are welcome to join for networking focused on career development.</p>
AFTER 8:00 PM	CORPORATE HOSPITALITY SUITES AT HILTON AMERICAS

THURSDAY, JUNE 8, 2023

7:00 AM	CORPORATE BREAKFAST SEMINARS , Convention Center
7:30 AM - 2:00 PM	NAME BADGE PRINTING & INFORMATION , Level One Lobby (outside Hall B)
8:30 - 10:30 AM	<p>ORAL SESSIONS</p> <p>ThOA am: Instrumentation: Ambient Ionization and Applications, Hall B3 ThOB am: Glycopeptides, Glycoproteins, and Glycomics, Grand Ballroom A ThOC am: Metabolomics: Untargeted Profiling, Grand Ballroom B ThOD am: Data-Independent Acquisition and Multiplexing: Proteomics, Grand Ballroom C ThOE am: Fundamentals Beyond Mass Analysis: Structural Characterization of Isomers, Room 332 ThOF am: Protein-Ligand and Protein-Protein Interactions, General Assembly A ThOG am: Microbes and the Microbiome, General Assembly B ThOH am: Nucleic Acids and Oligonucleotides, General Assembly C</p>
10:30 AM - 2:30 PM	<p>POSTER SESSION AND EXHIBITS, Thursday Posters, Halls BC</p> <p>Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm</p>
2:30 - 4:30 PM	<p>ORAL SESSIONS</p> <p>ThOA pm: Instrumentation: Innovative Separation Approaches Coupled to MS, Hall B3 ThOB pm: Biotherapeutics: Proteins, Antibodies, and Antibody/Drug Conjugates, Grand Ballroom A ThOC pm: Imaging: Pharmaceuticals, Metabolites, Lipids, and Glycans, Grand Ballroom B ThOD pm: Fundamentals: Ion Structures and Energetics, Grand Ballroom C ThOE pm: Environmental: Innovative Approaches and Instrumentation, Room 332 ThOF pm: Lipidomics: Targeted and Untargeted, General Assembly A ThOG pm: Forensics: Innovations and Applications, General Assembly B ThOH pm: Informatics: Innovations, General Assembly C</p>
4:45 - 5:30 PM	<p>PLENARY LECTURE, Hall B3</p> <p>The Rise and Reign of the Mammals: A New History, from the Shadow of the Dinosaurs to Us</p> <p>Stephen Brusatte <i>University of Edinburgh</i></p>
7:00 – 10:00 PM	<p>CLOSING EVENT AT THE HOUSTON MUSEUM OF NATURAL SCIENCE</p> <p>Advance purchase ticket is required. Ticket sales CLOSE on Monday June 5, 12pm noon.</p> <p>Buy your ticket online via Online Registration portal (you can add-on to your existing conference registration). If you purchase after printing your name badge, you will need to re-print your badge.</p> <p>There is no organized transport to/from the event. Attendees with the closing event icon on their badge have round-trip light rail included. Please wear your badge in case there is ticket control. Engineers will identify your closing event icon as your paid ride. Light rail instructions are included in the app and will be emailed to all who have purchased the closing event.</p> <p>The Houston Museum of Natural Science is located at 5555 Hermann Park Drive, Houston TX 77030.</p> <p>If you do not wish to take the light rail, Uber/Lyft or taxis are available.</p>

MONDAY ORALS

MOA am: Top Down Protein Analysis Hall B3

Session Chair: Frederik Lermite (Technical University of Darmstadt)

- MOA am 08:30 **Proteoforms - how can we transfer them intact from tissues into mass spectrometers?**; Hartmut Schlüter¹; Jan Hahn¹; Manuela Moritz¹; Hannah Voss¹; Marcel Kwiatkowski²; ¹UKE - Section Mass Spectrometry and Proteomics, University of Hamburg, Hamburg, Germany; ²Functional Proteo-Metabolomics, Department of Biochemistry, University of Innsbruck, Innsbruck, Austria
- MOA am 08:50 **Native top-down for sequencing G protein-coupled receptors and related complexes directly from native membranes**; Corinne Lutomski^{1,2}; Tarick J El-Baba^{1,2}; Jack L Bennett^{1,2,3}; Sophie AS Lawrence^{1,2}; Joshua D Hinkle⁴; Ildir Liko⁵; Andrew Dolan^{1,2}; Christopher Mullen⁶; John E.P. Syka⁶; Carol V Robinson^{1,2}; ¹Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; ²University of Oxford, Oxford, United Kingdom; ³School of Chemistry, UNSW Sydney, Sydney, Australia; ⁴Thermo Fisher Scientific, San Jose, California; ⁵OMass Therapeutics, Oxford, United Kingdom; ⁶Thermo Fisher Scientific, San Jose, CA
- MOA am 09:10 **Native top-down mass spectrometry approaches to determine the FraB/FrIB-substrate binding sites and conformational changes induced by substrate binding**; Yuan Gao¹; Sravya Kovvali²; Jamison Law¹; Venkat Gopalan¹; Vicki H Wysocki¹; ¹The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; ²The Ohio State University-Department of Microbiology, Columbus, OH
- MOA am 09:30 **Parameter-free Deconvolution and Visualization of Peptide and Protein Fragmentation Mass Spectra**; Adrian L Guthals¹; Derrill Sturgeon¹; Alexander Gavrilenko¹; Blake Hakkila¹; Stephanie Sturgeon¹; Jhenya Gavrilenko¹; Rachel Franklin¹; Yury Vasil'ev¹; Joseph Meeuwse¹; Valery Voinov¹; Joseph Beckman¹; ¹e-MSion, Corvallis, OR
- MOA am 09:50 **Internal Fragment Assignment Challenges in Top-Down Electron Capture Dissociation Tandem Mass Spectrometry**; Neven N. Mikawy¹; Carolina Rojas Ramirez¹; Brandon T. Ruotolo¹; Kristina Hakansson¹; ¹University of Michigan, Ann Arbor, Michigan
- MOA am 10:10 **Unravelling proteoform footprints of proteasome subtypes using top-down mass spectrometry**; Angélique Sanchez Dafun¹; Dusan Zivkovic¹; Stephen Adonai Leon Icaza¹; Sophie Moeller²; Carine Froment¹; Delphine Bonnet^{3,4}; Adriana Almeida De Jesus⁵; Laurent Alric⁴; Muriel Quarant-Nicaise³; Audrey Ferrand³; Céline Cougoule¹; Etienne Meunier¹; Odile Burlet-Schiltz¹; Frédéric Ebstein²; Raphaëla Goldbach-Mansky⁵; Elke Krüger²; Marie-Pierre Bousquet¹; Julien Marcoux⁶; ¹IPBS Toulouse, Toulouse, France; ²Institute of Medical Biochemistry and Molecular Biology, University Medicine Greifswald, Greifswald, Germany; ³IRSD, Université de Toulouse, INSERM, INRA, INP ENVT, Université de Toulouse 3 Paul Sabatier, Toulouse, France; ⁴Internal medicine department of digestive disease, Rangueil Hospital, Université de Toulouse III - Paul Sabatier (UPS), Toulouse, France; ⁵NIH/NIAID, Bethesda, MD; ⁶CNRS, Toulouse, France

MOB am: Imaging: Instrumentation & Method Development Ballroom A

Session Chair: Chris Anderton (Pacific Northwest National Lab)

- MOB am 08:30 **Enhancements in the use of water secondary ion mass spectrometry (SIMS) for multi-omic biomolecular mass and structural analysis**; Felicia M Green¹; Sadia Sheraz^{1,2}; Elena Castellani^{1,3}; Zoltan Takats^{1,4}; Nick Lockyer²; ¹Rosalind Franklin Institute, Harwell, Didcot, United Kingdom; ²University of Manchester, Manchester, United Kingdom; ³University of Oxford, Dept. of Chemistry, Oxford, United Kingdom; ⁴Imperial College London, London, United Kingdom
- MOB am 08:50 **Design and performance characterisation of a novel MALDI-2-MSI ionisation source with transmission and reflective mode capabilities**; Andrej Grgic¹; Benjamin Bartels¹; Alexandros Lekkas²; Diamantis Kounadis²; Elias Panagiotopoulos²; Dimitris Papanastasiou²; Ron M.A. Heeren¹; Shane R. Ellis^{1,3,4}; ¹M4i - Maastricht MultiModal Molecular Imaging Institute, Maastricht University, Maastricht, Netherlands; ²Fasmatech, NCSR Demokritos, Athens, Greece; ³Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; ⁴Illawarra Health and Medical Research Institute, Wollongong, Australia
- MOB am 09:10 **Multimodal IR-Guided MALDI Imaging of Biological Samples at High Spatial Resolution**; Ethan Yang¹; Peng Wang²; Joshua L Fischer¹; Thomas Tague²; Marten Seeba³; Hans-Christian Koch³; Tim Rider²; Katherine Stumpo¹; Michael Easterling¹; ¹Bruker Daltonics, Billerica, MA; ²Bruker Optics Inc, Billerica, MA; ³Bruker Optics GmbH & Co. KG, Ettlingen, Germany
- MOB am 09:30 **Harnessing the Power of Unit Resolution: Separating Isobars and Isomers using Tandem Mass Spectrometry Imaging**; Miranda R. Weigand¹; Daisy M. Unsuhay Vila¹; Manxi Yang¹; Hang Hu¹; Shane Tichy²; Julia Laskin¹; ¹Purdue University, Dept. of Chemistry, West Lafayette, IN; ²Agilent Technologies, Santa Clara, CA
- MOB am 09:50 **Probing Spatially Resolved Intact Macromolecular Complexes and Proteoforms Directly from Tissue using Native and Denatured Proteoform Imaging Mass Spectrometry**; Vijaya Lakshmi Kanchustambham¹; Pei Su¹; Jared O. Kafader¹; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL
- MOB am 10:10 **DESI imaging at the cellular level through the application of nano-flow and multi-focus approaches**; Emrys A Jones¹; Emmy Hoyes²; Scott Trinkle³; Richard Chapman⁴; ¹Waters, Wilmslow, United Kingdom; ²Waters Corporation, Wilmslow, United Kingdom; ³Waters, Milford, MA; ⁴Waters Corporation, Milford, MA

MOC am: Clinical Analysis: Innovations Ballroom B

Session Chair: Jennifer Van Eyk (Cedars Sinai Medical Center)

- MOC am 08:30 **Structural Characterization of Non-Microbial Ions in Urinary Tract Infections by MALDI-TOF MS Lipidomics**; Linda K Nartey¹; Abanoub Mikhael¹; Helena Petrosova¹; Michael X Chen²; Robert K Ernst³; David R Goodlett¹; ¹University of Victoria, Victoria, BC; ²UBC, Vancouver, BC; ³University of Maryland, Baltimore, MD
- MOC am 08:50 **Rapid LC-MS/MS First-Tier Newborn Screening Assay with Throughput Equivalent to FIA-MS/MS**; Samantha L Isenberg¹; C. Austin Pickens¹; Adrienne Manning²; Carla Cuthbert¹; Konstantinos Petritis¹; ¹Centers for Disease Control and Prevention, Atlanta, GA; ²Katherine A. Kelley State Public Health Laboratory, Rocky Hill, CT

MONDAY ORALS

- MOC am 09:10 **Rapid ICP-MS Analysis of Dried Blood Spots via Direct Microextraction from Solid Substrates;** R. Kenneth Marcus¹; Cameron J. Stouffer¹; ¹*Clemson University, Clemson, SC*
- MOC am 09:30 **A generic loading strategy for automated sample loading of Evtotips for robust and high throughput analysis on the Evosep One;** Magnus Huusfeldt¹; Dorte B. Bekker-Jensen¹; Jacob Poder¹; Moritz Heusel¹; Lasse Falkenby¹; Nicolai Bache¹; ¹*Evosep, Odense, Denmark*
- MOC am 09:50 **On-site Breast Cancer Diagnosis Using Paper Spray Ionization Miniature Mass Spectrometry;** Cheng-Chih Hsu¹; Hou-Chun Huang¹; Hsin-Hsiang Chung¹; Jia-Ying Yu¹; Bo-Rong Chen²; Ming-Yang Wang²; ¹*Department of Chemistry, National Taiwan University, Taipei City, Taiwan;* ²*Department of Surgery, National Taiwan University Hospital, Taipei City, Taiwan*
- MOC am 10:10 **Spatial chemistry of the developing brain with defective mitochondria;** Carlos Rodriguez-Navas¹; Md Amir Hossen²; Mohamed Boutaghou²; Arif Kocabas¹; Manuel Gonzalez¹; Isaac Marin-Valencia¹; ¹*Icahn School of Medicine at Mount Sinai, New York, NY;* ²*Shimadzu Scientific Instrument, Columbia, MD*

MOD am: Small Molecules: Structural Characterization and Quantitation Ballroom C

Session Chair: Athula Attygalle (Stevens Institute of Technology)

- MOD am 08:30 **Why do we fail structural analysis of organic compounds based on spectral appearance? Reflections on a few natural products' cases;** Takemichi Nakamura¹; Toshihiko Nogawa¹; ¹*RIKEN, Wako, Japan*
- MOD am 08:50 **Structural Characterization of Small Molecules Using Modelling and an Advanced Fragmentation Model;** Bela Paizs^{1,2}; Zoltan Takats^{2,3,4}; ¹*Rosalind Franklin Institute, Didcot, United Kingdom;* ²*deshape ltd, London, United Kingdom;* ³*Rosalind Franklin Institute, Harwell, Didcot, United Kingdom;* ⁴*Imperial College, London, United Kingdom*
- MOD am 09:10 **The present and future of Orbitrap-based, natural-abundance, high-precision isotope measurements in life science studies;** John M Eiler; *California Institute of Technology, Pasadena, CA*
- MOD am 09:30 **Isomeric Characterization of Illicit Drugs Using High-Resolution Linear and Differential Ion Mobility Separations;** Atena Tajaddodi¹; Hayden Thurman¹; Billy Kantharidis²; Alexandre A. Shvartsburg¹; Gavin E. Reid^{2,3,4}; ¹*Wichita State University, Wichita, KS;* ²*School of Chemistry, The University of Melbourne, Parkville, Australia;* ³*Department of Biochemistry and Pharmacology, The University of Melbourne, Parkville, Australia;* ⁴*Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Parkville, Australia*
- MOD am 09:50 **Structural elucidation of conjugation drug metabolites by utilizing novel electron-activated dissociation (EAD);** Ming Yao¹; Qian Ruan¹; ¹*Bristol-Myers Squibb, Princeton, NJ*
- MOD am 10:10 **Analysis of Thyroxine enantiomers in Pharmaceuticals by Ion Mobility Analysis based on molecular complexes;** Fangling Wu¹; Chuan-Fan Ding²; ¹*Ningbo University, Ningbo, China;* ²*Ningbo University, Ningbo, China*

MOE am: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements Room 332

Session Chair: Lorna De Leoz (Agilent Technologies)

- MOE am 08:30 **Gas phase cationization for pesticide analysis: charge-solvated vs. protonated salt for cypermethrin diastereomers distinction under resonant excitation conditions;** Kam Eng Trinh¹; Sophie Liuu²; Chenqin Cao³; Ekaterina Darii⁴; Jean-Claude Tabet^{3,5}; Annelaure Damont³; François Fenaille³; Olivier Firmesse²; Jacques-Antoine Hennekinne²; Chanthadary Inthavong¹; Gwenaelle Lavison-Bompard¹; ¹*Pesticides and Marine Biotoxins unit (PBM), Laboratory for Food Safety, French Agency for Food, Environmental and Occupational Health & Safety (ANSES), Université Paris-Est, Maisons-Alfort, 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*CEA-INRA, Laboratoire Innovations en Spectrométrie de Masse pour la Santé (LI-MS), DRF / Institut Joliot / DMTS / SPI, MetaboHUB, CEA Saclay - Université Paris Saclay, Gif-sur-Yvette, France;* ⁴*Génomique métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Université Evry, Université Paris-Saclay, Evry, France;* ⁵*Faculté des Sciences et de l'Ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Sorbonne Université, Paris, France*
- MOE am 08:50 **Distinguishing between common mold types in mandarins by SPME-SICRIT-MS;** Taylor Hayward¹; Allie Ferranti¹; Thomas Wolf²; Jan-Christoph Wolf²; ¹*Plasmion, Skillman, NJ;* ²*Plasmion, Augsburg, Germany*
- MOE am 09:10 **A machine learning method for predicting the origin of biological foreign substances from spectra acquired by MALDI TOF MS;** Hiroki Saito; *Asahi Quality & Innovations. Ltd., Moriya, Japan*
- MOE am 09:30 **Monitoring Global Soybean Production Using Elementomics to Combat Rainforest Destruction;** Brian Quinn¹; Yunhe Hong¹; Nicholas Birse¹; Chris Elliott¹; ¹*Queen's University Belfast, Belfast, United Kingdom*
- MOE am 09:50 **A comparative untargeted metabolomics analysis of açai (Euterpe oleracea Mart.) fruit, food powder, and botanical dietary supplement extracts;** Kabre L. Heck¹; Lauren E. Fogel¹; Yuyan Yi²; Jingyi Zheng²; Angela I. Calderon¹; ¹*Department of Drug Discovery and Development, Auburn University, Auburn, AL;* ²*Department of Mathematics and Statistics, Auburn University, Auburn, AL*
- MOE am 10:10 **--Characterizing Bourbon Whiskey via the Combination of LC-MS and GC-MS Based Molecular Fingerprinting;** Rui Xu¹; Hong Chen¹; Huan Zhang^{1,2}; Michael W. Crowder²; Jiangjiang Zhu¹; ¹*The Ohio State University, Columbus, OH;* ²*Miami University, Oxford, OH*

MOF am: Covalent Labeling and Chemical Crosslinking General Assembly A

Session Chair: Richard Scheltema (Utrecht University)

- MOF am 08:30 **Custom isobaric labeling strategies for quantitative chemoproteomics;** Kerian Backus¹; Nikolas Burton²; Flowreen Shikwana²; Daniel Polasky³; Samuel Ofori²; Daniel Geiszler³; Alexey I Nesvizhskii³; ¹*UNIVERSITY OF CALIFORNIA LOS ANGELES, Los Angeles, CA;* ²*UCLA, Los Angeles, CA;* ³*University of Michigan-Ann Arbor, Ann Arbor, MI*
- MOF am 08:50 **Cryo-XL: sub-zero in situ crosslinking on cryo-fixed cells under organic solvents;** Bruno C. Amaral¹; Andrew R. M. Michael¹; Raja S. Kondrapolu²; Darin E. Jones²; David C. Schriemer¹; ¹*University of Calgary, Calgary, AB;* ²*University of Arkansas for Medical Sciences, Little Rock, AR*

MONDAY ORALS

MOF am 09:10 **Footprinting integral membrane proteins in their native environment;** Jie Sun¹; Mierxiati Saimi²; Qing Cao²; Don L. Rempel¹; Mengqi Chai³; Weikai Li²; Michael L. Gross¹; ¹Washington University in St. Louis, St. Louis, MO; ²Washington University School of Medicine, St. Louis, MO; ³Washington university in St Louis, St Louis, MO

MOF am 09:30 **qXL-MS elucidation of membrane protein unfolding to visualize membrane complexes dynamics;** Anna Bakhtina¹; Sung-Gun Park¹; Martin M. Mathay¹; James E. Bruce¹; ¹University of Washington, Seattle, WA

MOF am 09:50 **Defining the Structures and Interactions of the Human Platelet Secretome using Chemical Crosslinking;** Michelle Cielesh¹; Jemma Fenwick¹; Fay Ghani¹; Yvonne Kong¹; Freda H Passam¹; Mark Larance¹; ¹Charles Perkins Centre, University of Sydney, Sydney, Australia

MOF am 10:10 **Characterizing Glycan-Induced Structural Changes and Binding Interfaces for IgG1-C1q Complex using Hydroxyl Radical Protein Footprinting;** Emily Chea¹; Zhi Cheng¹; Jiana Duan¹; Tyler Fletcher¹; Scot Weinberger¹; ¹GenNext Technologies, Half Moon Bay, CA

**MOG am: Polymers
General Assembly B**
Session Chair: Anthony Gies (Dow Chemical)

MOG am 08:30 **Characterization of Macrocyclic and Ring Architectures by Collision Induced Unfolding;** Calum Bochenek¹; Kayla N Williams-Pavlantos¹; Andrew S McGee¹; Chrys Wesdemiotis¹; ¹The University of Akron, Akron, OH

MOG am 08:50 **Assessing Degradability of Poly(Lactic-co-Glycolic Acid) Chains using Reactive Desorption Electrospray Ionization Mass Spectrometry;** Laurence Charles¹; Thierry NJ Fouquet²; Jean-Arthur Amalian³; Isaure Sergent⁴; Pierre Giusti^{5, 6}; Didier Gigmes⁴; ¹Aix-Marseille University, Marseille Cedex 20, France; ²Bausch+Lomb, Rochester, NY; ³Sanofi, Aramon, France; ⁴Aix Marseille Université, CNRS, Institut de Chimie Radicalaire, MARSEILLE, France; ⁵TotalEnergies OneTech R&D, TotalEnergies Research & Technology, Gonfreville, France; ⁶International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harfleur, France

MOG am 09:10 **The MS/MS of the dendrimers, hyperbranched polymers, and linear polymers of bis-MPA;** Scott M. Grayson¹; Mckenna J. Redding¹; Kayla N Williams-Pavlantos²; Oluwapelumi O. Kareem¹; Chrys Wesdemiotis²; ¹Tulane University, New Orleans, LA; ²University of Akron, Akron, OH

MOG am 09:30 **Characterization of Modified Hyaluronic Acid Materials and Their Interaction with Contact Lenses;** Michelle L. Piotrowski¹; Andrew J. Hotelling¹; ¹Bausch+Lomb, Rochester, NY

MOG am 09:50 **LDI-TOF MS and Graphical Data Analysis of Mesophase Pitch Samples used in Carbon Fiber Production;** Mark A Arnould¹; Aparna Annamraju²; Ercan Cakmak²; Frederic Vautard²; ¹Bruker Scientific, LLC, Billerica, MA; ²Oak Ridge National Laboratory, Oak Ridge, TN

MOG am 10:10 **Structural identification of PET (Polyethylene terephthalate) insoluble polyester polymers and microplastics by chemical depolymerization & advanced mass spectrometry;** Bayan Almasri^{1, 2}; Ahmed Mazzah¹; Youssef Bakkour^{2, 3}; Christian Rolando^{1, 4}; ¹Miniaturization for Synthesis, Analysis & Proteomics (MSAP), USR 3290, CNRS, University of Lille, Faculty of Sciences & Technologies, 59655 Villeneuve d'Ascq cedex, France; ²Laboratory of

Applied Chemistry (LAC), Lebanese University, Faculty of Sciences, Tripoli, Lebanon; ³College of Applied Medical Sciences, King Khalid University, Abha, Saudi Arabia; ⁴Shrieking Sixties, 1-3 Allée Lavoisier, 59650 Villeneuve d'Ascq, France

**MOH am: Informatics: Metabolomics and Lipidomics
General Assembly C**

Session Chair: Corey Broeckling (Colorado State University)

MOH am 08:30 **Network Topology Construction for Molecular Networking;** Xianghu Wang¹; Mingxun Wang²; ¹University of California, Riverside, riverside, CA; ²University of California, Riverside, Riverside, CA

MOH am 08:50 **An Automated Workflow Composition System In LC-MS Metabolomics Data Processing;** Xinsong Du¹; Farhad Dastmalchi¹; Matthew A. Diller¹; Mathias Brochhausen²; Timothy J. Garrett¹; William R. Hogan¹; Dominick J. Lemas¹; ¹University of Florida, Gainesville, FL; ²University of Arkansas for Medical Sciences, Little Rock, AR

MOH am 09:10 **Comparing the Use of Internal Standards Against Other Approaches for Normalization of LC-MS Lipidomics Data;** Kelly Stratton¹; Rachel Richardson¹; Jennifer E. Kyle¹; Josie G. Eder¹; Kristin M Engbrecht¹; Athena A. Schepmoes¹; Bobbie-Jo Webb-Robertson¹; Lisa M Bramer¹; ¹Pacific Northwest National Laboratory, Richland, WA

MOH am 09:30 **A Machine Learning Model for Chemical Formula Prediction Using Tandem Mass Spectra of Compounds;** Yuhui Hong¹; Haixu Tang¹; ¹Indiana University Bloomington, Bloomington, IN

MOH am 09:50 **Development of Aggregated Molecular Phenotype (AMP) Scores to Associate and Visualize Molecular Changes;** Jessie Chappel¹; Mary King²; Rachel Dehoog²; Livia S. Eberlin²; David Reif³; Erin S. Baker⁴; ¹North Carolina State University, Raleigh, NC; ²Baylor University, Waco, TX; ³National Institute of Environmental Health and Sciences, Raleigh, North Carolina; ⁴University of North Carolina at Chapel Hill, Chapel Hill, NC

MOH am 10:10 **Reaction-centered multi-omics integration of metabolomics data for mechanistic hypothesis generation;** Nikolai Köhler¹; Vivian Würf¹; Josch K Pauling¹; ¹LipiTUM, Technical University of Munich, Freising, Germany

MOH pm 02:30 **Speeding up proteomics using a micro-flow LC timsTOF-HT;** Johanna Tüshaus¹; Claire Delbridge²; Eike Mucha³; Christoph Krisp⁴; Jürgen Schlegel²; Bernhard Kuster¹; ¹Technical University of Munich, Freising, Germany; ²Technical University of Munich, Munich, Germany; ³Bruker Daltonics GmbH & Co.KG, Bremen, Germany; ⁴Bruker Dalton's GmbH & Co KG, Bremen, Germany

MONDAY ORALS

MOA pm: Single Cell Omics Hall B3

Session Chair: Yu Gao (University of Illinois, Chicago)

- MOA pm 02:30 **Single-shape proteomics with an ultra-high sensitivity workflow and preserving spatial context in organs;** Matthias Mann^{1, 2}; Florian A. Rosenberger¹; Marvin Thielert¹; Maximilian T. Strauss²; Katherine Madden¹; Constantin Ammar¹; Sophia C. Maedler¹; Lisa Schweizer¹; Andreas Metousis¹; Patricia Skowronek¹; Maria Wahle¹; Edwin Rodriguez¹; Thierry M. Nordmann¹; Andreas Mund²; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark
- MOA pm 02:50 **Using single cell mass spectrometry to evaluate CRISPR/Cas9 gene editing results;** Tra D Nguyen¹; Lindsie Martin¹; Zongkai Peng¹; Rakhi Rajan¹; Zhibo Yang¹; ¹University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK
- MOA pm 03:10 **Capturing Cardiomyocyte Cell-to-Cell Heterogeneity via Shotgun Top-Down Proteomics;** Fabio P. Gomes¹; Blandine Chazarin²; Aleksandra Binek²; Jolene K. Diedrich¹; Jennifer E. Van Eyk²; John R. Yates III¹; ¹Scripps Research, La Jolla, CA; ²Advanced Clinical Biosystems Research Institute, The Smidt Heart Institute, Cedars Sinai Medical Center, Los Angeles, CA
- MOA pm 03:30 **Robust label-free single-cell proteome analysis through in-capillary sample preparation (inCapS);** Adela-Eugenie Vrsanova¹; Syed Azmal Ali¹; Mathias Kalxdorf²; Jeroen Krijgsveld¹; ¹German Cancer Research Center, Heidelberg, Germany; ²Cellzome GmbH (a GSK company), Heidelberg, Germany
- MOA pm 03:50 **Electrophoresis-Correlative Mass Spectrometry Enables Ultrasensitive Proteomics;** Bowen Shen¹; Peter Nemes¹; ¹University of Maryland, College Park, College Park, MD
- MOA pm 04:10 **Sensitive and robust high-throughput workflow for qualitative and quantitative single-cell/single cell like analysis;** Tabiwang N. Arrey¹; Bernard Delanghe¹; Santosh Renuse²; Jeff Op De Beeck³; Paul Jacobs³; Nicolaie Eugen Damoc¹; ¹Thermo Fisher Scientific, Bremen, Germany; ²Thermo Fisher Scientific, San Jose, California; ³Thermo Fisher Scientific - Belgium, Ghent, Belgium

MOB pm: Ion Mobility: Instrumentation & Method Development Ballroom A

Session Chair: Hélène Lavanant (Université de Rouen Normandie)

- MOB pm 02:30 **Use of dendrimers to calibrate ion mobility cross section measurements;** Jens Sommertune¹; Emily R. Sekera²; Bela Paizs³; Zoltan Takats³; Arpad Somogyi²; ¹Polymer Factory Sweden, Stockholm, Sweden; ²The Ohio State University, Columbus, OH; ³Rosalind Franklin Institute, Harwell, Didcot, United Kingdom
- MOB pm 02:50 **Hydrazide derivatization in conjunction with cyclic ion mobility-based collision cross section measurements for the improved characterization of human milk oligosaccharides;** Sanaz C Habibi¹; Gabe Nagy¹; ¹University of Utah, Salt Lake City, UT
- MOB pm 03:10 **Development of an Array of Ion Traps in Structures for Lossless Ion Manipulations (SLIM);** Adam P. Huntley¹; Adam L. Hollerbach¹; Aneesh S. Prabhakaran¹; Cameron M. Giberson¹; Randolph V. Norheim¹; Richard D. Smith¹; Yehia M. Ibrahim¹; ¹Pacific Northwest National Laboratory, Richland, WA
- MOB pm 03:30 **Leveraging High-Resolution Separations with Selective SLIM-IMS Ion-Neutral**

Clustering, HDX, and Cryogenic IR Spectroscopy; Vasyl Yatsyna¹; Brian H Clowers²; Thomas Rizzo¹; ¹Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland; ²Washington State University Department of Chemistry, Pullman, WA

MOB pm 03:50 **Native mass spectrometry on a modified timsTOF Pro;** Yu-Fu Lin¹; Angela Di Capua¹; Erin Panczyk²; Benjamin Jones²; Mark Ridgeway²; Arpad Somogyi¹; Desmond Kaplan³; Melvin Park²; Vicki Wysocki¹; ¹The Ohio State University, Columbus, OH; ²Bruker Daltonics, Billerica, MA; ³KapScience LLC, TEWKSBURY, MA

MOB pm 04:10 **Investigating the effect of high field inelastic collisions using a DMA-FAIMS Hybrid Method for Improved Ion Mobility characterization;** Viraj D Gandhi^{1, 2}; Jihyeon Lee³; Christopher J. Hogan³; Carlos Larriba-Andaluz⁴; ¹Indiana University Purdue University - Indianapolis, Indianapolis, IN; ²Purdue University, Lafayette, IN; ³University of Minnesota, Minneapolis, MN; ⁴Indiana University Purdue University Indianapolis, Indianapolis, IN

MOC pm: Structural Biology Ballroom B

Session Chair: Lan Huang (University of California, Irvine)

- MOC pm 02:30 **In-cell Crosslinking Mass Spectrometry combined with AlphaFold-Multimer to discover and predict the structures of novel protein complexes;** Francis J O'Reilly¹; Andrea Graziadei^{2, 3}; Christian Forbrig²; Rica Bremenkamp⁴; Jörg Stülke⁴; Juri Rappsilber^{1, 2}; ¹NCI NIH, Frederick, MD; ²Technische Universität Berlin, Berlin, Germany; ³Human Technopole, Milan, Italy; ⁴University of Göttingen, Göttingen, Germany
- MOC pm 02:50 **An integrative structural interactomics approach to reveal protein organization, topology and structure of intact Giant virus particles;** Lars Muehlberg¹; Boris Bogdanow¹; Kenta Okamoto²; Liu Fan¹; ¹Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; ²Uppsala University, Uppsala, Sweden
- MOC pm 03:10 **Deciphering the mode of interaction for novel insulin receptor partial agonists by HDX-MS and cryo-EM;** Haihong Zhou¹; Giovanna Scapin¹; Yacob Gomez Llorente¹; Terri Kelly¹; David McLaren¹; Songnian Lin¹; James Mu¹; ¹Merck & Co., Inc., Kenilworth, New Jersey
- MOC pm 03:30 **Unravelling the Mechanism of Rotavirus Viral Factory Formation using Structural Mass Spectrometry;** Alice Colyer¹; Julia Acker²; Xinyu Wang²; Alexander Borodavka²; Antonio Calabrese¹; ¹University of Leeds, Leeds, United Kingdom; ²University of Cambridge, Cambridge, United Kingdom
- MOC pm 03:50 **Direct determination of membrane protein complexes from cellular membranes;** Wonhyeuk Jung¹; Aniruddha Panda¹; Kallol Gupta¹; ¹Yale School of Medicine, Department of Cell Biology, New Haven, CT
- MOC pm 04:10 **Barcoded nanobodies for the capture and characterization of native membrane protein complexes from human brain;** Tarick J El-Baba^{1, 2}; Corinne A Lutomski^{1, 2}; Jack L Bennett^{1, 3, 4}; Sophie AS Lawrence^{1, 3}; Andrew Dolan^{1, 2}; Idir Liko⁵; Joshua D Hinkle⁶; Christopher Mullen⁷; John E.P. Syka²; Carol V Robinson^{1, 2}; ¹Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; ²Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom; ³Department of Chemistry, University of Oxford, Oxford, United Kingdom

MONDAY ORALS

Kingdom; ⁴School of Chemistry, UNSW Sydney, Sydney, Australia; ⁵OMass Therapeutics, Oxford, United Kingdom; ⁶ThermoFisher Scientific, San Jose, CA; ⁷Thermo Fisher Scientific, San Jose, CA

MOD pm: Data-Independent Acquisition and Multiplexing: Lipidomics and Metabolomics

Ballroom C
Session Chair: TBD

- MOD pm 02:30 **Untargeted and Targeted DIA-SWATH Mass Spectrometry for the Characterization of Metabolite and Xenobiotics in Pediatric Chronic Kidney Disease Urine Samples;** María Fernanda Cifuentes Girard¹; Gérard Hopfgartner¹; ¹University of Geneva, Geneva, Switzerland
- MOD pm 02:50 **Deep Structural Lipidomics using Ozone-Induced Dissociation in a High-Throughput Data-Independent Analysis Workflow;** Jesse A Michael¹; Alan T Maccarone¹; Todd W Mitchell¹; Christer S Ejsing^{2, 3}; Shane R. Ellis¹; ¹School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; ²Department of Biochemistry and Molecular Biology, Villum Center for Bioanalytical Sciences, University of Southern Denmark, Odense, Denmark; ³Cell Biology and Biophysics Unit, European Molecular Biology Laboratory, Heidelberg, Germany
- MOD pm 03:10 **Creating Deconvoluted Open-Source Files from Data-Independent Analysis Files using IonDecon;** Nandarani Abril¹; Jeremy Koelmel²; Michael Kummer¹; Ralph Hindle³; Kathy Hunt³; Stephan Baumann⁴; Krystal J Godri Pollitt²; Emma E Rennie⁴; ¹Innovative Omics, Sarasota, FL; ²Yale University, New Haven, CT; ³Vogon Labs, Cochrane, Alberta; ⁴Agilent Technologies, Santa Clara, CA
- MOD pm 03:30 **Analysis of yeast lipids exposed to low temperature stress using data-independent acquisition-based lipidomics;** Daiki Hara¹; Nobuyuki Okahashi^{2, 3}; Atsuhiko Toyama⁴; Junko Iida^{3, 5}; Fumio Matsuda^{2, 3}; ¹Osaka University, Suita, Japan; ²Osaka University, Suita, Osaka, Japan; ³Osaka University Shimadzu Omics Innovation Research Laboratories, Suita, Japan; ⁴Shimadzu Corporation, Kyoto, Japan; ⁵SHIMADZU Corporation, Kyoto, Japan
- MOD pm 03:50 **A powerful single method for sensitive quantification and targeted/non-targeted identification of cell culture media (CCM) components using accurate mass spectrometry;** Marialuca Maldini¹; Antonella Chiapparino²; Eshani Nandita³; ¹SCIEX, Milano, Italy; ²SCIEX, Darmstadt, Germany; ³SCIEX, Redwood City, CA
- MOD pm 04:10 **Plasma Lipidomics using diaPASEF Demonstrates Improved Capabilities of Quantification using MS2 Data;** Premy Shanthamoorthy¹; Hannes Roest¹; ¹University of Toronto, Toronto, ON

- MOE pm 02:50 **Novel mass spectrometry method for the detection and quantification of peanut protein in processed food matrices;** Sara K Schlange¹; Justin T Marsh¹; Melanie L Downs¹; Philip E Johnson¹; ¹University of Nebraska-Lincoln, Lincoln, NE
- MOE pm 03:10 **Isotopologue ratio analysis in organic compounds: caffeine in complex sample matrices;** Nils Johannes Kuhlbusch^{1, 2}; Dieter Juchelka³; Issaku Edward Kohl³; Andreas Hilkert³; Heiko Hayen¹; ¹University of Muenster, Muenster, Germany; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ³Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- MOE pm 03:30 **A novel reactomic platform to retrieve reactive carbonyl species (RCS) and their interaction with polyphenols;** Changling Hu¹; Miao Yu²; Yantao Zhao¹; Yingdong Zhu¹; Shengmin Sang¹; ¹North Carolina A&T State University, Kannapolis, NC; ²The Jackson Laboratory, Bar Harbor, ME
- MOE pm 03:50 **Cooking food in microwavable plastic containers: in situ formation of a new chemical substance and increased migration of polypropylene polymers;** Francisco José Díaz-Galiano¹; María José Gómez-Ramos¹; Iciar Beraza-Gómez¹; María Murcia-Morales¹; Amadeo Rodríguez Fernández-Alba¹; ¹University of Almería, Department of Chemistry and Physics, Agrifood Campus of International Excellence (ceiA3), Almería, Spain
- MOE pm 04:10 **Regioselective dissociation by collisional activation of alkali-cationized cereulide in gas phase, coexisting charge-solvated vs. protonated salt forms;** Sophie Liuu¹; Kam Eng Trinh²; Chenqin Cao³; Ekaterina Darii⁴; Annelaure Damont³; Jean-Claude Tabet^{3, 5}; Yves Gimbert⁶; François Fenaille³; Yassine Makni²; Chanthadary Inthavong²; Gwenaëlle LAVISON-BOMPARD²; Jacques-Antoine Hennekinne¹; Olivier Firmesse¹; ¹Staphylococcus, 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; ²Pesticides and Marine Biotoxins unit (PBM), Laboratory for Food Safety, French Agency for Food, Environmental and Occupational Health & Safety (ANSES), Université Paris-Est, Maisons-Alfort, France; ³CEA-INRA, Laboratoire Innovations en Spectrométrie de Masse pour la Santé (LI-MS), DRF / Institut Joliot / DMTS / SPI, MetaboHUB, CEA Saclay - Université Paris Saclay, Gif sur Yvette, France; ⁴Génomique métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry, France; ⁵Faculté des Sciences et de l'Ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Sorbonne Université, Paris, France; ⁶Département de Chimie Moléculaire, UMR CNRS 5250, Université Grenoble Alpes, Grenoble, France

MOE pm: Food Safety & Chemistry: Innovations Room 332

Session Chair: Boniek Vaz (Universidade Federal de Goiás, Brazil)

- MOE pm 02:30 **Photoionization MS as tool to predict product sensory information as well as physical and chemical product attributes in real time;** Jan Heide^{1, 2}; Hendryk Czech²; Sven Ehlert¹; Andreas Walte¹; Ralf Zimmermann^{2, 3}; ¹Photonion GmbH, Schwerin, Germany; ²Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; ³Department for Science and Technology of Life, Light and Matter (LL&M), University of Rostock, Rostock, Germany

MOF pm: Cancer Research General Assembly A

Session Chair: Sarah Totten (Lycia Therapeutics)

- MOF pm 02:30 **Immunopeptidomics identifies tumor associated antigens in pancreatic ductal adenocarcinoma---;** Eva Verzani¹; Zackery Ely²; Karl R Clauser¹; Susan Klaeger¹; Zachary Kulstad²; Andrew Aguirre^{1, 3, 4}; William A Freed-Pastor^{2, 4}; Jennifer G Abelin¹; Tyler Jacks²; Steven A Carr¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²Massachusetts Institute of Technology, Cambridge, Massachusetts; ³Harvard Medical School, Boston, MA; ⁴Dana-Farber Cancer Institute, Boston, MA

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- MOF pm 02:50 **Proteoform Imaging Mass Spectrometry to Interrogate the Ovarian Cancer Microenvironment**; Nathaniel Henning^{1, 2}; Vijaya Lakshmi Kanchustambham^{1, 2}; Pei Su^{1, 2}; Michael Caldwell^{1, 2}; Jared O. Kafader^{1, 2}; Thomas Conrads³; Neil L. Kelleher^{1, 2}; ¹*Chemistry of Life Processes Institute, Northwestern University, Evanston, IL*; ²*The Proteomics Center of Excellence, Northwestern University, Chicago, IL*; ³*Women's Health Integrated Research Center at Inova Health System, Annandale, Virginia*
- MOF pm 03:10 **Characterization of Metabolic Variabilities Associated to Glioblastoma to Identify Patient Specific Combination Therapies using Liquid Chromatography-Tandem Mass Spectrometry**; Stellena Mathiaparanam¹; Olga Zaslaver¹; Michelle Kushida^{1, 2}; Trevor Pugh^{1, 3}; Peter Dirks^{1, 2}; J. Rafael Montenegro-Burke¹; Hannes Röst¹; ¹*University of Toronto, Toronto, ON*; ²*The Hospital for Sick Children, Toronto, ON*; ³*Princess Margaret Cancer Centre, Toronto, ON*
- MOF pm 03:30 **Employing Top-down Mass Spectrometry to Examine RAS Proteoforms in Malignant Cell Lines**; Caroline Dehart¹; Robert A. D'ippolito¹; Kanika Sharma¹; Nicole Fer¹; Brian Smith¹; Mackenzie Meyer¹; Scott Eury¹; Abigail Neish¹; Katie Powell¹; Vanessa Wall¹; William Burgan¹; Dominic Esposito¹; Anna E. Maciag¹; Frank McCormick^{1, 2}; Dwight V. Nissley¹; ¹*Frederick National Laboratory for Cancer Research, Frederick, MD*; ²*Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA*
- MOF pm 03:50 **Hepatic Steatosis Induced by Bioactive Lipids**; Mario M Alba¹; Ielyzaveta Slarve¹; Brandon Ebright¹; Whitaker Cohn²; Yiren Zhou¹; Jared Khan¹; Yuni Jia¹; Aditi Datta¹; Lina He¹; Taojian Tu¹; Pranav Pammidimukkala¹; Phillip Nguyen¹; Jonathan Katz^{1, 3}; Julian Whitelegge²; Stan Louie¹; Bangyan Stiles¹; ¹*USC, Los Angeles, CA*; ²*UCLA, Los Angeles, CA*; ³*The Lawrence J Ellison Institute for Transformative Medicine of USC, Los Angeles, CA*
- MOF pm 04:10 **Optimization of peptide purification and DDA-PASEF method for increased sensitivity of MHC class II peptide identification**; Raghothama Chaerkady¹; Li Dai¹; Kristina Archer¹; Abby J. Chiang¹; Lisa H Cazares¹; Rajat Varma¹; Mark Cobbold¹; Sonja Hess¹; ¹*AstraZeneca R&D, Gaithersburg, Maryland*
- MOG pm 03:50 **Machine learning-derived charge state assignments with better accuracy than human experts**; Heather Desaire¹; David Hua¹; Hanna Nguyen¹; Eden Go¹; ¹*University of Kansas, Lawrence, KS*
- MOG pm 04:10 **Faster CDMS: Unusual Charge Detection Mass Spectrometry (CDMS) Methods for Rapid Analysis of MDa-sized Analytes**; Zachary M. Miller¹; Conner C. Harper¹; Evan R. Williams¹; ¹*University of California, Berkeley, Berkeley, CA*
- MOH pm: High Throughput MS
General Assembly C**
Session Chair: John Tran (Genentech)
- MOH pm 02:50 **Robust and High-Throughput Analytical Flow Proteomics Analysis of Cynomolgus Monkey and Human Matrices with Zeno SWATH Data Independent Acquisition**; Weiwun Sun¹; Yuan Lin¹; Yue Huang¹; Joselyn Chan¹; Sonia Terrillon¹; Anton I. Rosenbaum¹; Kevin Contrepois¹; ¹*AstraZeneca, South San Francisco, CA*
- MOH pm 03:10 **One-minute proteome analysis using a novel high-resolution accurate mass platform**; Trenton M Peters-Clarke¹; Tabiwang N. Arrey²; Lia Serrano¹; Noah M Lancaster¹; Anna Pashkova²; Evgenia Shishkova¹; Michael S. Westphall¹; Christian Hock²; Nicolaie Eugen Damoc²; Vlad Zabrouskov³; Joshua J. Coon^{1, 4}; ¹*University of Wisconsin-Madison, Madison, WI*; ²*Thermo Fisher Scientific, Bremen, Germany*; ³*Thermo Fisher Scientific, San Jose, California*; ⁴*Morgridge Institute for Research, Madison, WI*
- MOH pm 03:30 **Next generation high-throughput multiplexed chemoproteomics in 96-well plates on a high resolution accurate mass platform with a new mass analyzer**; Qing Yu¹; Ka Yang¹; Kevin Dong¹; Martin Zeller²; Graeme C McAlister³; Joao A Paulo¹; Hamish Stewart²; Christian Hock²; Nicolaie Eugen Damoc²; Vlad Zabrouskov³; Steven P Gygi¹; ¹*Harvard Medical School, Boston, MA*; ²*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*; ³*Thermo Fisher Scientific, San Jose, CA*
- MOH pm 03:50 **Ultra-high-throughput Intact Protein Analysis for Drug Discovery Using Acoustic Ejection Mass Spectrometry**; Xiujuan Wen¹; Kiersten Tovar¹; Adway O. Zacharias¹; Chang Liu²; Richard Johnstone¹; Ryan Loy¹; Lyle Burton²; Thomas R. Covey²; Markus Koglin¹; Kevin P. Bateman³; Mary Jo Wildey¹; David G. McLaren¹; ¹*Merck & Co., Kenilworth, NJ*; ²*SCIEX, Concord, ON*; ³*Merck, West Point, PA*
- MOH pm 04:10 **High Throughput Mass Spectrometry for Biopharma: An Orthogonal and Complementary Analytical Method for Characterization and Relative Quantitation of Multispecific Antibodies**; Iain D G Campuzano¹; Fuyi Chen¹; Dhanashri Bagal²; Dwight Winters¹; Christopher Spahr¹; Emma Pelegri-O'Day²; Nithya Srinivasan¹; Jennifer L Lippens¹; Pascal Egea³; Aiko Umeda¹; Jennifer Aral¹; Tianqi Zhang⁴; Arthur Laganowsky⁴; Marissa Mock¹; Chawita Netirojanakul¹; ¹*Amgen, Thousand Oaks, CA*; ²*Amgen, South San Francisco, CA*; ³*UCLA, Los Angeles, CA*; ⁴*Texas A&M University, College Station, TX*
- MOG pm: Fundamentals: Unconventional Approaches in MS
General Assembly B**
Session Chair: Leslie Hicks (University of North Carolina, Chapel Hill)
- MOG pm 02:30 **Miniature, Monolithic, Fully Additively Manufactured Glass-Ceramic Quadrupole Mass Filters for Portable Mass Spectrometry**; Colin Eckhoff¹; Nicholas K. Lubinsky¹; Luis F. Velasquez-Garcia¹; ¹*MIT, Cambridge, MA*
- MOG pm 02:50 **Real-time Pressure Control Algorithm Enables Vacuum Design for Miniature mass spectrometer**; Ningxi Li¹; Zhijun Cai¹; Xiaoyu Zhou¹; Zheng Ouyang¹; ¹*Tsinghua University, Beijing, China*
- MOG pm 03:10 **The Wisconsin Oscillator: A Low-Cost Circuit for Powering Ion Guides, Traps, Funnels, and Ion Mobility Spectrometers**; Steven J Kregel¹; Blaise J. Thompson¹; Gilbert M. Nathanson¹; Timothy H. Bertram¹; ¹*University of Wisconsin-Madison, Department of Chemistry, Madison, WI*
- MOG pm 03:30 **Mass Spectrometer Observing Lunar Operations (MSolo)**; Roberto Aguilar Ayala¹; Matthew L. Hancock¹; Alexander W. Jarnot^{1, 2}; Janine E. Captain¹; Jacqueline W. Quinn¹; ¹*National Aeronautics and Space Administration, Kennedy*

TUESDAY ORALS

TOA am: Instrumentation: New Developments in Ionization and Sampling (In Memory of Marvin Vestal)

Hall B3

Session Chair: Brian Musselman (Bruker)

- TOA am 08:30 **Electroless ionization mass spectrometry (ELI-MS), a plug-and-play ambient technique for ultrasoft ionization;** Stefan Kooij¹; Aleksandra Chojnacka²; Garry L. Corthals²; Cees Van Rijn³; ¹*Van der Waals Zeeman Institute, Amsterdam, Netherlands*; ²*Van t Hoff Institute for Molecular Sciences, Amsterdam, Netherlands*; ³*Van der Waals Zeeman Institute, Amsterdam, Netherlands*
- TOA am 08:50 **MS SIEVE – pushing the limits for low-abundant (bio)molecules;** Nina Morgner¹; Kudratullah Karimi¹; Jonathan Zöller²; Tommy Hofmann³; Rene Zangl¹; Jonathan Schulte¹; Carla Schmidt^{3, 4}; Julian D Langer²; ¹*Goethe-University, Institute of Physical and Theoretical Chemistry, Frankfurt am Main, Germany*; ²*Proteomics, Max-Planck-Institute for Brain Research, Frankfurt am Main, Germany*; ³*HALOmem, Institute of Biochemistry and Biotechnology, Martin Luther University Halle-Wittenberg, Halle, Germany*; ⁴*Department of Chemistry – Biochemistry, Johannes Gutenberg University Mainz, Mainz, Germany*
- TOA am 09:10 **DON'T SLEEP ON SAMPLING – IF YOU DON'T GRAB IT YOU CAN'T SEE IT;** Dan Carmany¹; Paul Demond^{2, 3}; Patrick W. Fedick⁴; Elizabeth Dhummakupt²; ¹*Excet, Gunpowder, MD*; ²*U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD*; ³*EXCET Incorporated, Edgewood, MD*; ⁴*Naval Air Warfare Center, United States Navy Naval Air Systems Command (NAVAIR), China Lake, CA*
- TOA am 09:30 **Miniaturized plasma-based ionization source for LC-MS detection of multiclass explosives;** Priscilla Rocio Bautista¹; Marcos Bouza Areces²; Sebastian Brandt³; Joachim Franzke³; Antonio Molina Díaz^{2, 4}; Juan Francisco García Reyes^{2, 4}; ¹*Universidad de Jaén, Jaén, Spain*; ²*University of Jaén, Jaén, Spain*; ³*ISAS- Leibniz Institut für Analytische Wissenschaften, Dortmund, Germany*; ⁴*University Research Institute for Olives Grove and Olive Oil, University of Jaén, Jaén, Spain*
- TOA am 09:50 **The newly designed "Aim" soft chemical ionization reactor for direct, real-time measurement of inorganic acids, organics, and PFAS in air;** Abigail Koss¹; Matthieu Riva²; Felipe Lopez-Hilfiker²; ¹*Tofwerk USA, Boulder, CO*; ²*Tofwerk AG, Thun, Switzerland*
- TOA am 10:10 **cVSSI-APCI-MS for rapid identification of drugs and their metabolites in serum;** Madison Pursell¹; Liam P. Poole²; Kaitlyn J. Apgar¹; Stephen Valentine²; Peng Li²; ¹*West Virginia University, Morgantown, WV*; ²*West Virginia University- C. Eugene Bennett Department of Chemistry, Morgantown, WV*

TOB am: Biomarkers: Quantitative Analysis

Ballroom A

Session Chair: Norelle Wildburger (AstraZeneca)

- TOB am 08:30 **Histone post-translational modifications as determinants for drug outcome in T-cell acute lymphoblastic leukemia;** Laura Corveleyn¹; Lien Provez²; Bart Van Puyvelde¹; Dieter Deforce¹; Pieter Van Vlierberghe²; Maarten Dhaenens¹; ¹*Lab of Pharmaceutical Biotechnology, Ghent University, Ghent, Belgium*; ²*Department of Biomolecular Medicine, Ghent University, Ghent, Belgium*
- TOB am 08:50 **Absolute quantification of IgA1 immune-complex proteins in serum of patients with IgA**

nephropathy; Mary A. Cunningham¹; Ellenore P. Craine¹; Alyssa L. Hansen¹; Stacy Hall¹; Dana V. Rizk¹; Bruce A. Julian¹; Jan Novak¹; Matthew B. Renfrow¹; ¹*University of Alabama at Birmingham, Birmingham, AL*

- TOB am 09:10 **Quantitative Analysis of GCASE Activity in DBS: Working Towards Decentralizing the Patient Clinical Trial Experience;** Brendan Tierney¹; Ting-Wen Cheng¹; Savon Vigil¹; Matthew Blatnik¹; ¹*Pfizer, Groton, CT*
- TOB am 09:30 **Ultra-fast SARS-CoV-2 peptide detection using peptide-immunoaffinity enrichment combined with Acoustic Ejection Mass Spectrometry (AEMS);** Bart Van Puyvelde¹; Christie Hunter²; Yang Oliver Wang³; Esthelle Hoedt³; Maxim Zhgamadze³; Koen Raedschelders³; Qin Fu³; Dieter Deforce¹; Maarten Dhaenens¹; Jennifer Van Eyk³; ¹*Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium*; ²*SCIEX, Redwood City, CA*; ³*Cedars-Sinai Medical Center, Los Angeles, CA*
- TOB am 09:50 **D-Amino Acids Quantification by LC-MS/MS-MRM in Type 1 Diabetes-Affected Human Serum;** Shuangshuang Chen¹; Cindy J. Lee¹; Stanislav S. Rubakhin¹; Jonathan V. Sweedler¹; ¹*University of Illinois Urbana Champaign, Urbana, IL*
- TOB am 10:10 **A Blood-Based Lipid Biomarker Panel For Personalized Risk Assessment of Breast Cancer;** Johannes Fahrman¹; Ehsan Irajizad¹; Jody Vykoukal¹; Angelica Gutierrez Barrera¹; Jennifer B Dennison¹; Ranran Wu¹; Banu Arun¹; Abenaa Brewster¹; Samir Hanash¹; ¹*MD Anderson, Houston, TX*

TOC am: Fundamentals: Native MS and Structures of Large Ions

Ballroom B

Session Chair: Boris Krichel (University of Siegen / CSSB Hamburg)

- TOC am 08:30 **Native Top-Down MS with Orbitrap-Based Electron Capture Dissociation Reveals Higher Order Structure Information for Protein Complexes;** Boyu Zhao¹; Carter Lantz¹; Benqian Wei¹; Rachel R. Ogorzalek Loo¹; Joseph A. Loo¹; ¹*University of California, Los Angeles, Los Angeles, CA*
- TOC am 08:50 **Sensitive characterization of native protein complexes from biological samples using biofunctionalized dissolvable hydrogel microbeads;** Xinyang Shao^{1, 2}; Yanyi Huang^{1, 2}; Guanbo Wang^{1, 2}; Jianbin Wang³; ¹*Peking University, Beijing, China*; ²*Shenzhen Bay Laboratory, Shenzhen, China*; ³*Tsinghua University, Beijing, China*
- TOC am 09:10 **MS analysis of free, circulating 20S-proteasomes from blood;** Gili Ben-Nissan¹; David Morgenstern¹; Yegor Leushkin¹; Michal Sharon¹; ¹*Weizmann Institute of Science, Rehovot, Israel*
- TOC am 09:30 **Can We Really Correctly Assign Charge States of Large Oligomeric Complexes? Spectral Interferences in Native MS of Macromolecular Assemblies;** Victor Yin¹; Janet C Saunders²; Paul WA Devine²; Nicholas J Bond²; Albert J.R. Heck¹; ¹*Utrecht University, Utrecht, Netherlands*; ²*AstraZeneca, Cambridge, United Kingdom*
- TOC am 09:50 **Unleashing the power of CE-MS: from the separation of ~1 MDa multimeric protein assembly conformers to their in-depth structural characterization;** Anne-Lise Marie¹; Somak Ray¹; Alexander R. Ivanov¹; ¹*Barnett Institute of Chemical and Biological Analysis, Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA*

TUESDAY ORALS

TOC am 10:10 **In-Line Soft Landing for Cryo-EM and Mass Spectrometry Characterization of Hydrated Native Complexes and Glycoproteins;** Elizabeth Duselis¹; Henry Benner²; Ben Aguilar²; Ananya Dubey Kelsoe²; Matthew Johnson¹; Wayne Fairbrother¹; Alexis Rohou¹; Elizabeth Hecht¹; ¹Genentech, South San Francisco, CA; ²IonDX Inc., Monterey, CA

**TOD am: Informatics: Peptide and Protein Identification, Proteomics
Ballroom C**

Session Chair: Olga Vitek (Northeastern University)

TOD am 08:30 **Detecting and removing interference in precursor quantification;** Brian C. Searle^{1, 2}; Ariana E Shannon¹; Damien B Wilburn¹; ¹The Ohio State University, Columbus, OH; ²Proteome Software, Portland, OR

TOD am 08:50 **A systematic characterization of LC-MS features sheds light on the full potential of DIA identification;** Grzegorz Skoraczyński¹; Tejas Gandhi¹; Oliver M Bernhardt¹; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland

TOD am 09:10 **Library-free analysis of DIA experiments using a feature-centric approach;** J. Sebastian Paez¹; Carolyn Allen¹; Lindsay K Pino¹; Daniele Canzani¹; William E Fondrie¹; ¹Talus Bioscience, Seattle, WA

TOD am 09:30 **Fragment ion intensity prediction improves the identification rate of non-tryptic peptides in TimsTOF;** Charlotte Adams¹; Wassim Gabriel²; Kris Laukens¹; Wout Bittremieux¹; Mathias Wilhelm²; Kurt Boonen¹; ¹University of Antwerp, Antwerpen, Belgium; ²Technical University of Munich, Munich, Germany

TOD am 09:50 **A modular and open workflow for the extraction and quantification of peptides in synchro-PASEF experiments;** Georg Wallmann¹; Patricia Skowronek²; Marvin Thielert²; Corazon Ericka Mae Itang¹; Sander Willems^{3, 4}; Wen-Feng Zeng¹; Matthias Mann^{1, 5}; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Max Planck Institute of Biochemistry, Martinsried, Germany; ³Max Planck Institute of Biochemistry, Planegg, Germany; ⁴Bruker Daltonics, Bremen, Germany; ⁵NNF Center for Protein Research, University of Copenhagen, Copenhagen, Denmark

TOD am 10:10 **SEPeQuant enables comprehensive protein isoform characterization in shotgun proteomics;** Yongchao Dou^{1, 2}; Xinpei Yi^{1, 2}; Lindsey k Olsen^{1, 2}; Bing Zhang^{1, 2}; ¹Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; ²Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX

**TOE am: Exposomics, Toxicology, and Health Outcomes
Room 332**

Session Chair: Yinsheng Wang (University of California, Riverside)

TOE am 08:30 **Exposomic approaches for next-generation human biomonitoring;** Benedikt Warth; *University of Vienna, Vienna, Austria*

TOE am 08:50 **Medication Read-out in Untargeted Metabolomics Using a MS/MS Library of Drugs and Metabolites Propagated from Repository-scale Molecular Networking;** Haoqi Nina Zhao¹; Wout Bittremieux^{1, 2}; Corinna Brungs³; Robin Schmid^{1, 3}; Simone Zuffa¹; Pieter C Dorrestein¹; ¹University of California San Diego, San Diego, CA; ²University of Antwerp, Antwerpen, Belgium; ³Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic

TOE am 09:10 **Development of a sensitive high-resolution LC-MS/MS approach for global profiling of urinary mercapturic acid conjugates;** Kevin Murray^{1, 2}; Dylan McKeon¹; Chiara Lecchi¹; Peter W. Villalta¹; Silvia Balbo¹; ¹Masonic Cancer Center, University of Minnesota, Minneapolis, MN; ²Center for Metabolomics and Proteomics, University of Minnesota, Minneapolis, MN

TOE am 09:30 **Detecting temporal changes in the serum albumin adductome following bariatric surgery using Pan-Protein Adductomics;** Joshua W Smith¹; Robert N O'Meally²; Sean M Burke¹; Robert H Brown^{1, 3}; John D Groopman¹; Robert N Cole²; ¹Department of Environmental Health and Engineering, Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD; ²Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD; ³Department of Anesthesiology, School of Medicine, Johns Hopkins University, Baltimore, MD

TOE am 09:50 **Chemical exposome in brain cancer: An exploratory study;** Ruben Gil-Solsona¹; Albert Pons-Escoda²; Daniel Gutierrez-Martin¹; Jordi Bruna^{3, 3}; Noemi Vidal-Sarro⁴; Carles Majos²; Pablo Gago Ferrero¹; ¹Institute of Environmental Assessment and Water Research - Spanish Council for Scientific Research (IDAEA-CSIC), Barcelona, Spain; ²Department of Neuroradiology, Hospital Universitari de Bellvitge, C. Feixa Llarga SN, 08907 L'Hospitalet de Llobregat, Spain, Hospitalet de Llobregat, Spain; ³Unit of Neuro-Oncology, Hospital Universitari de Bellvitge-ICO, Barcelona, Spain; ⁴Neuropathology Institute, Hospital Universitari de Bellvitge, Barcelona, Spain

TOE am 10:10 **Assessing Per- and Polyfluoroalkyl Substances (PFAS) and Lipidomic Alterations in Plants Grown in Contaminated Soil;** Rebecca L Beres¹; Sarah Doydora²; Kaylie I Kirkwood³; Allen Li⁴; Owen Duckworth²; Erin S Baker¹; ¹Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; ²Department of Crop and Soil Sciences, North Carolina State University, Raleigh, NC; ³Department of Chemistry, North Carolina State University, Raleigh, NC; ⁴Institute of Plant Protection, Chinese Academy of Agricultural Sciences, Beijing, China

**TOF am: Neurodegenerative Disease Research
General Assembly A**

Session Chair: Judith Steen (Boston Children's Hospital)

TOF am 08:30 **Multi-omics profiling of human induced pluripotent stem cells (iPSCs) to investigate the mechanisms of splicing dysfunction in AD pathogenesis;** Zhen Wang¹; Ping-Chung Chen¹; Junmin Peng¹; ¹St. Jude Children's Research Hospital, Memphis, TN

TOF am 08:50 **Mass spectrometry reveals ATP production defects in Niemann-Pick disease, type C1 mouse brain myelin and human oligodendrocytes;** Chandimal Pathmasiri¹; Stephanie M Cologna¹; ¹University of Illinois at Chicago, Chicago, IL

TOF am 09:10 **Machine Learning Models Predict Mild Traumatic Brain Injury Using Lipid Mass Spectrometry Imaging Data;** Dmitry Leontyev¹; Alexis N Pulliam²; David A Gaul¹; Michelle C Laplaca²; Facundo M Fernandez¹; ¹School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; ²Coulter Department of Biomedical Engineering, Georgia Institute of Technology/Emory University, Atlanta, GA

TOF am 09:30 **Analysis of Brain Protein Stability Changes in Mouse Models of Normal Aging and Alzheimer's**

TUESDAY ORALS

- TOF am 09:50 **Disease; Yun Tang¹; Hyejin Park¹; Michael C. Fitzgerald¹; ¹Duke University, Durham, NC**
- TOF am 10:10 **BrainProt: An Omics based knowledgebase towards the understanding of Human Brain and diseases; Deeptharup Biswas¹; Sanjyot Vinayak Shenoy¹; Aparna Chauhan¹; Advait Padhye¹; Sanjeeva Srivastava¹; ¹IIT Bombay, Mumbai, India**
- TOF am 10:10 **Employing LCMS/MS-based system-wide quantification of N-glycosylation to determine the effects of fatty acids on a neuroinflammation cell model; Sheryl Joyce B. Grijaldo^{1,2}; Michael Russelle S. Alvarez²; Ryan Lee Schindler²; Armin Oloumi²; Tristan Alexander Seales²; Siyu Chen²; Nikita P. Bacalzo, Jr.²; Jorge Gil C. Angeles¹; Francisco M. Heralde III³; Jomar F. Rabajante¹; Ruel C. Nacario¹; Gladys C. Completo¹; Carlito B. Lebrilla²; ¹University of the Philippines Los Banos, Los Banos, Laguna, Philippines; ²University of California, Davis, Davis, CA; ³University of the Philippines Manila, Manila, Philippines**

**TOG am: Drug Metabolism and Pharmacokinetics
General Assembly B
Session Chair: Josh Yu (Gilead)**

- TOG am 08:30 **Automated High-Resolution Mass Spectrometry Data Processing Meets/Beats QQQ for Drug Quantification Studies; Kevin Bateman¹; Fabien Fontaine²; Bernard Choi¹; Luca Moretoni³; Ismael Zamora²; ¹Preclinical Development, Merck Research Lab. Merck & Co., Inc, West Point, PA; ²Lead Molecular Design, S.L., Sant Cugat del Valles, Spain; ³Molecular Discovery, Elstree Borehamwood, United Kingdom**
- TOG am 08:50 **Confident characterization and identification of glucuronide metabolites using diagnostic fragments from orthogonal MS/MS data; Rahul Baghla¹; Eshani Nandita¹; ¹SCIEX, Redwood City, CA**
- TOG am 09:10 **Quantitative Analysis of Liver mARC1 in Different Species Using Reagent Free-Automatic High pH Fractionation Enrichment (RF-auto HpH) and LC-MS; Xue Dong¹; Julie Lade¹; Fang Xie¹; Zhe Wang¹; Xiaomeng Shen¹; ¹Amgen, Inc., South San Francisco, CA**
- TOG am 09:30 **Accelerator Mass Spectrometry @ Boehringer-Ingelheim – implementing ultrahigh sensitive 14C analysis for routine microtracer studies in DMPK; Ralf Lau¹; Stefan Blech²; ¹Boehringer Ingelheim Pharma, Biberach, Germany; ²Boehringer Ingelheim Pharma, Biberach, Germany**
- TOG am 09:50 **Intact Protein Mass Analysis throughout Covalent Drug Discovery, including Pharmacokinetics/Pharmacodynamics, Tissue Distribution, Route of Administration, Dose Estimation, and Efficacy; Md Amin Hossain¹; Rutali R. Brahme¹; Brandon C. Miller¹; Jakal Amin¹; Jared R. Auclair¹; Qingping Wang²; David J. Greenblatt³; Roman Manetsch¹; Jeffrey N. Agar¹; ¹Northeastern University, Boston, MA; ²Sanofi, Cambridge, MA; ³School of Medicine, Tufts University, Boston, MA**
- TOG am 10:10 **Quantitative Proteomics supports characterization of complex translational in vitro models for oral prodrugs; Xue Wang¹; Liang Jin¹; Abhinav Sharma²; David Stresser²; Yu Tian¹; ¹AbbVie Bioresearch Center, Worcester, MA; ²AbbVie Inc., North Chicago, IL**

**TOH am: Imaging: Spatially-Resolved Omics
General Assembly C**

Session Chair: Elizabeth Neumann (University of California, Davis)

- TOH am 08:30 **Exploring cellular heterogeneity within human pancreas by 3D-MALDI imaging of intact proteoforms; Kevin J Zemaitis¹; Dušan Veličković¹; David J Degnan¹; James M Fulcher¹; Lye Meng Markille¹; Yu Mi Kwon¹; Dehong Hu¹; Yen-Chen Liao¹; Sarah M Williams¹; Lisa M Bramer¹; Ying Zhu¹; William Kew¹; Wei-Jun Qian¹; Mowei Zhou¹; Ljiljana Paša-Tolić¹; ¹Pacific Northwest National Laboratory, Richland, WA**
- TOH am 08:50 **Spatial Proteomics of the Skeletal Matrix in Osteoarthritis via MALDI-MSI Reveals Molecular Delineations in Disease Severity and New Biomarkers; Charles A. Schurman¹; Nannan Tao²; Jonathon J. Woo³; Tamara Alliston³; Peggi M. Angel⁴; Birgit Schilling¹; ¹Buck Institute for Research on Aging, Novato, CA; ²Bruker Daltonics, San Jose, CA; ³University of California San Francisco, Department of Orthopaedic Surgery, San Francisco, CA; ⁴Medical University of South Carolina, Charleston, SC**
- TOH am 09:10 **Deep Visual Proteomics and spatial transcriptomics uncover the landscape of tumor malignancy in borderline ovarian cancer; Lisa Schweizer¹; Rahul Krishnan²; Aasa Shimizu²; Andreas Metousis¹; Hilary Kenny²; Lisha Zhu²; Thierry Nordmann¹; Florian Rosenberger¹; Agnes Julia Bilecz⁴; Rachelle Mendoza⁴; Sanaa Nakad Borrego²; Marvin Thielert¹; Sophia Mäder¹; Andreas Mund⁵; Mengjie Chen³; Ricardo Lastra⁴; Matthias Mann^{1,5}; Ernst Lengyel²; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Department of Obstetrics and Gynecology/Section of Gynecologic Oncology, University of Chicago, Chicago, Illinois; ³Medicine/Section of Genetic Medicine, The University of Chicago, Chicago, Illinois; ⁴Department of Pathology, The University of Chicago, Chicago, Illinois; ⁵Proteomics Program, Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark**
- TOH am 09:30 **Correlating Tissue Biomechanics and Molecular Information – The Combination of physiological AFM and MALDI MSI; Martina Marchetti-Deschmann¹; Martin Handelshausen¹; Aleksandra Lebedeva¹; Orestis Andriotis¹; Philipp Thurner¹; ¹TU Wien, Vienna, Austria**
- TOH am 09:50 **MALDI Imaging of Post-Mortem COVID-19 Lungs; Caitlin Tressler¹; Gargey B. Yagnik²; Karl Smith^{3,4}; Nicole M. Jenkinson¹; Chad Weisbord⁴; Kenneth J. Rothschild²; Mark J. Lim²; David Nauen¹; Kristine Glunde¹; ¹Johns Hopkins University School of Medicine, Baltimore, MD; ²AmberGen, Inc., Billerica, MA; ³Leibniz-Institut für Analytische Wissenschaften—ISAS—e.V., Dortmund, Germany; ⁴National High Magnetic Field Laboratory, Tallahassee, FL**
- TOH am 10:10 **Software workflow and statistical analysis tools for evaluating multiomics MALDI MSI studies; Tobias Boskamp¹; Sören-Oliver Deininger¹; Mark Lim²; Gargey Yagnik²; Nathalie Agar³; Sylwia Stopka³; Richard R. Drake⁴; Stacy A. Malaker⁵; Rachel Stubler⁴; Kenneth J. Rothschild^{2,6}; ¹Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ²AmberGen, Inc., Billerica, MA; ³Harvard Medical School, Boston, MA; ⁴Medical University of South Carolina, Charleston, SC; ⁵Yale University, New Haven, CT; ⁶Boston University, Dept. of Physics and Photonics Center, Boston, MA**

TUESDAY ORALS

TOA pm: Instrumentation: High-Resolution Mass Spectrometry Hall B3

Session Chair: Ljiljana Pasa-Tolic (Pacific Northwest National Lab)

- TOA pm 02:30 **Enhanced resolving power using multiple passes of a multi-reflecting time-of-flight mass analyser; William Johnson¹**; Martin E. Palmer¹; Peter Nixon¹; Jason Wildgoose¹; ¹Waters Corporation, Wilmslow, United Kingdom
- TOA pm 02:50 **Pushing the boundaries of quantitative proteomics with data independent acquisition using a novel high-resolution accurate mass analyzer; Lilian R. Heil¹**; Nicolaie Eugen Damoc²; Tabiwang N. Arrey²; Anna Pashkova²; Chris Hsu¹; Christine C. Wu¹; Philip M Remes³; Hamish Stewart²; Christian Hock²; Michael Senko³; Vlad Zabrouskov³; Michael J. MacCoss¹; ¹University of Washington, Seattle, WA; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ³Thermo Fisher Scientific, San Jose, CA
- TOA pm 03:10 **Combining TIMS-ToF and FT-ICR: A prototype TIMS-FT-ICR MS instrument capable of deep characterisation of complex samples; Christopher Andrew Wootton¹**; Alina Theisen¹; Gregory Brabeck¹; Carlos Schat¹; Claudia Kriete¹; Roland Jertz¹; ¹Bruker Daltonics, Bremen, Germany
- TOA pm 03:30 **High Resolution Analysis of Megadalton Sized DNA using Charge Detection Mass Spectrometry; Lohra Miller¹**; Polycarp Ooegbu¹; Benjamin Draper¹; Martin F. Jarrold¹; ¹Indiana University Bloomington, Bloomington, IN
- TOA pm 03:50 **A novel quaternary hybrid Q-Orbitrap-IT-FT-ICR mass spectrometry platform; Chad R. Weisbrod¹**; Jesse D. Canterbury²; John P Quinn¹; Lissa C Anderson¹; Amy M McKenna¹; Greg T Blakney¹; Michael W. Senko²; Christopher L. Hendrickson¹; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Thermo Fisher Scientific, San Jose, California
- TOA pm 04:10 **Performance demonstration of an in situ laser desorption/ionization Orbitrap mass spectrometer; Adrian Southard^{1, 2}**; Soumya Ray¹; Ricardo Arevalo, Jr.³; Ryan M. Danell^{2, 4}; Jacob D Graham²; Andrej Grubisic²; Cynthia L Gundersen⁵; Niko A Minasola⁵; Anthony W Yu²; Molly E Fahey²; Christelle Briois⁶; Laurent Thirkell⁶; Fabrice Colin⁶; ¹University of Maryland College Park, College Park, MD; ²NASA Goddard Space Flight Center, Greenbelt, MD; ³University of Maryland, College Park, College Park, MD; ⁴Danell Consulting, Winterville, NC; ⁵AMU Engineering, Miami, FL; ⁶LPC2E, Orleans, France

TOB pm: Post-translational Modifications: Qualitative & Quantitative Analysis Ballroom A

Session Chair: Amy Weeks (University of Wisconsin, Madison)

- TOB pm 02:30 **New High-Resolution Accurate Mass (HRAM) Platform Enables Rapid and Deep Human Phosphoproteomics; Noah M Lancaster^{1, 2}**; Trenton M Peters-Clarke^{1, 2}; Tabiwang N. Arrey³; Anna Pashkova³; Nicholas Arp^{4, 5}; Jing Fan^{4, 5, 6}; Evgenia Shishkova^{2, 7}; Michael S. Westphall^{2, 7}; Hamish Stewart³; Eugen Damoc³; Vlad Zabrouskov⁸; Joshua J. Coon^{1, 2, 4, 7}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI; ³Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ⁴Morgridge Institute for Research, Madison, WI; ⁵Cellular and Molecular Biology Graduate Program, University of Wisconsin-Madison, Madison, WI; ⁶Department of

Nutritional Sciences, University of Wisconsin-Madison, Madison, WI; ⁷National Center for Quantitative Biology of Complex Systems, Madison, WI; ⁸Thermo Fisher Scientific, San Jose, CA

- TOB pm 02:50 **A novel paradigm for kinase-associated disorders: Multiplexed phosphoproteomic analysis of kinase specificity rewiring in patient-derived samples of rare neurodevelopmental disorder; Danielle M Caefer¹**; Jeremy Balsbaugh¹; Jennifer Liddle¹; Anastasios Tzingounis¹; Daniel Schwartz¹; ¹University of Connecticut, Storrs, CT
- TOB pm 03:10 **Investigating T-cell Activation Using the Phosphorylation Integrated Thermal Shift Assay; Brandon M Gassaway¹**; Alison E. Ringel²; Emily M. Huntsman³; Jared L. Johnson³; Lewis C. Cantley³; Edward L Huttlin¹; Steven P Gygi¹; Marcia C. Haigis¹; ¹Harvard Medical School, Boston, MA; ²MIT, Cambridge, MA; ³Weill Cornell Medicine, New York, NY
- TOB pm 03:30 **Time-resolved deep ubiquitinome profiling for protein degraders; Ishwar Kohale¹**; Aman Makaju²; Han-Yin Yang¹; Bradford Gibson¹; Daryl N Bulloch¹; ¹Amgen, South San Francisco, CA; ²Amgen, Thousand Oaks, CA
- TOB pm 03:50 **A quantitative and site-specific atlas of the in vivo citrullinome reveals widespread existence of citrullination; Alexandra Stripp¹**; Ivo A Hendriks¹; Sara C Buch-Larsen¹; Jonas D Elsborg¹; Rebecca Kirsch¹; Nadezhda T Doncheva¹; Lars J Jensen¹; Maria Christophorou²; Michael L Nielsen¹; ¹NNF Center for Protein Research, Univ of Copenhagen, Copenhagen N, Denmark; ²Babraham Institute, Cambridge, United Kingdom
- TOB pm 04:10 **PTMeXchange : Globally harmonized re-analysis and sharing of data on post-translational modifications; Kerry A Ramsbottom¹**; Oscar M Camacho¹; Zhi Sun²; Emily Bowler-Barnett³; Jun Fan³; Ananth Surappa-Narayanappa³; Deepti Kundu³; Yasset Perez-Riverol³; Maria-Jesus Martin³; Juan Antonio Vizcaino³; Eric W. Deutsch²; Andrew R Jones¹; ¹University of Liverpool, Liverpool, United Kingdom; ²Institute for Systems Biology, Seattle, WA; ³EMBL's European Bioinformatics Institute (EMBL-EBI), Wellcome Genome Campus, Hinxton, United Kingdom

TOC pm: Fundamentals: Ionization Methods Ballroom B

Session Chair: Steve Valentine (West Virginia University)

- TOC pm 02:30 **Spontaneous Breakup of Charged Aqueous Nanodrops: Dynamics of Rayleigh Fission in the Submicron Range; Emeline Hanozin¹**; Conner C Harper¹; Matthew S. McPartlan¹; Evan R. Williams¹; ¹University of California Berkeley, Berkeley, CA
- TOC pm 02:50 **Modelling Protein Charging during Electrospray with Molecular Dynamics Protocol for Proton Exchange between Discrete Grotthuss Diffuse H3O+ and Proteins; Michael S Cordes¹**; Elyssia S. Gallagher¹; ¹Baylor University, Waco, TX
- TOC pm 03:10 **Transition metal identification and speciation by MALDI FT-ICR MS as salen complexes; Elena Giaretta¹**; Farah Salma^{1, 2}; Davide Corinti³; Caterina Bordin¹; Manal Ridany¹; Mariaelisa Crestoni³; Christian Rolando^{1, 4}; ¹Faculty of Sciences & Technologies, University of Lille, Villeneuve d'Ascq, France; ²Faculty of Science III, Lebanese University, Tripoli, Lebanon; ³Dipartimento di Chimica e Tecnologia del Farmaco, Sapienza - Università di Roma, Roma, Italy; ⁴Shrieking Sixties - 1-3 Allée Lavoisier, Villeneuve d'Ascq, France
- TOC pm 03:30 **Effect of gas-phase on reactant ions, ionization and fragmentation in dielectric barrier discharge**

TUESDAY ORALS

ionization; Markus Weber^{1, 2}; Christoph Haisch²; Jan-Christoph Wolf¹; ¹Plasmion GmbH, Augsburg, Germany; ²Technical University of Munich, Munich, Germany

TOC pm 03:50 **Unravelling the Mechanisms of Magic Number Custer Formation During Electrospray Ionization;** Lars Konermann¹; Yousef Haidar¹; Vida Alinezhad¹; Elnaz Aliyari¹; ¹Univ. of Western Ontario, London, ON

TOC pm 04:10 **Use of Acoustic Energy to Disrupt Exosomes for Direct Compositional Analysis by MS;** Ashton N Taylor¹; Cheyenne Sircher¹; Yuqi Huang¹; Venkat Bhethanabotla¹; Theresa Evans-Nguyen¹; ¹University of South Florida, Tampa, FL

Madison, WI; ⁴Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ⁵EMBL Australia and Garvan Institute of Medical Research, Darlinghurst, Australia; ⁶School of Biotechnology and Biomolecular Sciences, University of New South Wales, Sydney, Australia; ⁷Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI; ⁸Department of Microbiology and Ecosystem Science, University of Vienna, Vienna, Austria; ⁹Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON; ¹⁰Department of Molecular Genetics, University of Toronto, Toronto, ON

TOD pm: Informatics: Multiomics Integration and Applications Ballroom C

Session Chair: Sonja Hess (AstraZeneca)

TOD pm 02:30 **Multi-omic microsampling for the profiling of lifestyle-associated changes in health;** Xiaotao Shen¹; Ryan Kellogg¹; Daniel Panyard¹; Nasim Bararpour¹; Kevin Castillo¹; Brittany Lee-McMullen¹; Alireza Delfarah¹; Jessalyn Ubellecker¹; Sara Ahadi¹; Yael Rosenberg-Hasson¹; Ariel Ganz¹; Kevin Contrepois¹; Basil Michael¹; Ian Simms¹; Chuchu Wang¹; Daniel Hornburg¹; Michael Snyder¹; ¹Stanford University, Stanford, CA

TOD pm 02:50 **A tissue specific post-translational modification (PTM) map of human proteome;** Pathmanaban Ramasamy^{1, 2, 3, 4}; Hanne Devos^{1, 2}; Wim F. Vranken^{3, 4}; Lennart Martens^{1, 2}; ¹VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; ²Department of Biomolecular Medicine, Faculty of Health Sciences and Medicine, Ghent, Belgium; ³Interuniversity Institute of Bioinformatics in Brussels, ULB-VUB, Brussels, Belgium; ⁴Structural Biology Brussels, Vrije Universiteit Brussel, Brussels, Belgium

TOD pm 03:10 **ProtPipe: An informatic pipeline for mass spectrometry-based proteomics and peptidomics;** Ziyi Li^{1, 2}; Nicholas Johnson^{1, 2}; Syed Shah^{1, 2}; Cory A Weller^{1, 2}; Ying Hao¹; Jessica Roberts¹; Rahel Bezabih¹; Mark R. Cookson³; Michael E. Ward⁴; Andrew B. Singleton¹; Mike A. Nalls^{1, 2}; Yue A. Qi¹; ¹Center for Alzheimer's and Related Dementias, National Institutes of Health, Bethesda, MD; ²Data Tecnica International, Washington, DC; ³Laboratory of Neurogenetics, National Institute on Aging, National Institutes of Health, Bethesda, MD; ⁴National Institute of Neurological Disorders and Stroke, National Institutes of Health, Bethesda, MD

TOD pm 03:30 **Mass spectrometry-based multi-omics identifies sarcopenia-associated molecular landscape perturbations in rhesus monkey skeletal muscle;** Melissa R Pergande¹; Yutong Jin¹; Kalina J Rossler¹; Gary M Diffie¹; Rozalyn M Anderson¹; Ricki J Colman¹; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI

TOD pm 03:50 **Development of a Tumor Immunopeptidome database for T cell-based therapies;** Yulun Chiu¹; Ke Pan¹; Cassian Yee¹; ¹The University of Texas MD Anderson Cancer Center, Houston, TX

TOD pm 04:10 **Deep Human Proteome Sequencing for Global Detection of Mutations and Alternative Splicing;** Pavel Sinitcyn^{1, 2}; Alicia L. Richards^{3, 4}; Robert J. Weatheritt^{5, 6}; Dain R. Brademan^{2, 7}; Harald Marx^{3, 7, 8}; Jesse Meyer^{3, 7}; Michael S. Westphall^{3, 7}; Evgenia Shishkova^{3, 7}; Benjamin J. Blencowe^{9, 10}; Juergen Cox¹; Joshua J. Coon^{2, 3, 4, 7}; ¹Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Martinsried, Germany; ²Morgridge Institute for Research, Madison, WI; ³National Center for Quantitative Biology of Complex Systems,

TOE pm: Plants and Natural Products Room 332

Session Chair: Joshua Kellogg (Pennsylvania State University)

TOE pm 02:30 **Mass spectrometry-based untargeted metabolomics approaches for comprehensive structural annotation of bioactive metabolites from bushy cashew (Anacardium humile) fruits;** Gabriel Franco Dos Santos¹; Nerilson M Lima¹; Gesiane S Lima¹; Jussara V Roque¹; Gagan Preet²; Teresinha De Jesus A. S. Andrade³; Marcel Jaspars⁴; Boniek Gontijo¹; ¹Federal University of Goiás - UFG, Goiânia, Brazil; ²University of Aberdeen, Aberdeen Proving Ground, United Kingdom; ³GEOMAR Helmholtz Centre for Ocean Research Kiel, Kiel, Germany; ⁴federal Institute of Science and Technology of Maranhão, Timon, Brazil

TOE pm 02:50 **Identifying chia oil in Colonial Mexican art materials using multi-omics approaches;** Aleksandra Popowich¹; Jose Luis Lazarte Luna¹; Catherine Gilbert²; Monica Katz³; Ronda Kasl¹; Christopher Mason⁴; Caroline Tokarski²; Julie Arslanoglu¹; ¹Metropolitan Museum of Art, New York, NY; ²Institute of Chemistry and Biology of Membrane and NanoObjects (CBMN), CNRS UMR 5248 University of Bordeaux, Bordeaux, France; ³The Hispanic Society of America, New York, NY; ⁴Weill Cornell Medicine, New York, NY

TOE pm 03:10 **Pathogen-oriented platform for large-scale discovery of drug-like natural products discovers novel antifungal targeting urgent-threat drug-resistant Candidiasis;** Bahar Behsaz¹; Andrés Mauricio Caraballo-Rodríguez²; Pieter C Dorrestein²; Hosein Mohimani¹; ¹Carnegie Mellon University, Pittsburgh, PA; ²University of California San Diego, San Diego, CA

TOE pm 03:30 **Profiling of the Polyphenol Content of Honey and its Relationship to Geographical Origins using HPLC-MS/MS;** Kate Nyarko¹; Kaitlyn Boozer¹; Michael Greenlief¹; ¹University of Missouri-Columbia, Columbia, MO

TOE pm 03:50 **Single-protoplast and tissue-specific proteomics of agronomic-relevant plant systems using a nanodroplet processing platform;** Sarai M Williams¹; James M Fulcher¹; William Chrisler¹; Liyu Andrey¹; Lye Meng Markille¹; Vimal Kumar Balasubramanian¹; Mowei Zhou¹; Jaeho Song²; Gary Stacey²; Amy Marshall-Colon³; John Mullet⁴; Amirhossein H. Ahkami¹; Ljiljana Pasa-Tolic¹; Ying Zhu⁵; ¹Pacific Northwest National Laboratory, Richland, WA; ²University of Missouri, Columbia, MO; ³University of Illinois at Urbana-Champaign, Urbana, IL; ⁴Texas A&M University, College Station, TX; ⁵Genentech Inc., South San Francisco, CA

TOE pm 04:10 **Looking into the small and fragile – highly resolved, matrix-free MSI of the floating fern Azolla and its specialized metabolites;** Benjamin Bartels¹; Erbil Güngör²; Sara Tortorella³; Ismael Zamora⁴; Henriette Schlupeppmann²; Ron M.A.

TUESDAY ORALS

Heeren¹; Shane R. Ellis^{1, 5}; ¹*M4I, University Maastricht, Maastricht, Netherlands*; ²*Department of Biology, Utrecht University, Utrecht, Netherlands*; ³*Molecular Horizon s.r.l, Bettona, Italy*; ⁴*Lead Molecular Design, S.L., Sant Cugat del Valles, Spain*; ⁵*Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia*

TOF pm: Ion Mobility: Structure Determination & Applications General Assembly A

Session Chair: Thanh Do (University of Tennessee, Knoxville)

- TOF pm 02:30 **Solution and Gaseous Ensembles of α -Synuclein: Towards a Biophysical Understanding of "Unstructured" Protein IM/MS**; Melanie Cheung See Kit¹; Tyler C Cropley²; Frank Sobott³; Christian Bleiholder²; Ian K. Webb¹; ¹*Indiana University Purdue University Indianapolis, Indianapolis, IN*; ²*Florida State University, Tallahassee, FL*; ³*University of Leeds, Leeds, United Kingdom*
- TOF pm 02:50 **Cyclic ion mobility-mass spectrometry and electron capture dissociation probe dimerization of aggregation-prone IAPP**; Aisha Ben-Younis¹; Alexander Zhyvoloup¹; Hannah Britt¹; Daniel Raleigh^{1, 2}; Konstantinos Thalassinos¹; ¹*University College London, London, United Kingdom*; ²*Stony Brook University, Stony Brook, NY*
- TOF pm 03:10 **Temperature-dependent Structural Changes of the 20S Proteasome as Measured by Cyclic Ion Mobility Spectrometry-Mass Spectrometry**; Lucas W Henderson¹; Edie M. Sharon¹; Adam J Anthony¹; Sarah M. O'keefe¹; David E. Clemmer¹; ¹*Indiana University Bloomington, Bloomington, IN*
- TOF pm 03:30 **Ion Mobility – Mass Spectrometry Evaluates the Effects of Lipid Bilayers On Membrane Protein Structure and Stability**; Iliana Levesque¹; Aniruddha Panda²; Kallol Gupta²; Brandon T Ruotolo¹; ¹*University of Michigan, Ann Arbor, MI*; ²*Yale University, New Haven, CT*
- TOF pm 03:50 **Resolving regio- and stereo-isomer complexity using cyclic ion mobility coupled to mass spectrometry**; Stephen J Blanksby¹; Berwyck Poad¹; Reuben S. E. Young^{1, 2}; Lachlan Jekimovs¹; Felicia Hansen¹; Thi Phuong Do¹; Hendrik Frisch¹; Michael Pfrunder¹; David L Marshall¹; Kathleen Mullen¹; ¹*Queensland University of Technology, Brisbane, Australia*; ²*University of Wollongong, Wollongong, Australia*
- TOF pm 04:10 **High-Resolution Ion Mobility Mass Spectrometry in Separation of Oligonucleotide Impurities**; Nnenna E Dieke¹; Joshua Shipman¹; Cynthia Sommers¹; Jason Rodriguez¹; Deyi Zhang²; Darby Kozak²; Kui Yang¹; ¹*U.S. Food and Drug Administration, Saint Louis, MO*; ²*U.S. Food and Drug Administration, Silver Spring, MD*

TOG pm: H/D Exchange: Innovations and Applications General Assembly B

Session Chair: Martial Rey (Institut Pasteur)

- TOG pm 02:30 **Folding of prestin's anion-binding site and implications to electromotility and hearing as revealed by HDX-MS**; Xiaoxuan Lin¹; Patrick Haller^{1, 2}; Navid Bavi^{1, 2}; Nabil Faruk¹; Eduardo Perozo^{1, 2, 3, 4}; Tobin R Sosnick^{1, 4, 5}; ¹*Department of Biochemistry and Molecular Biology, The University of Chicago, Chicago, IL*; ²*Center for Mechanical Excitability, The University of Chicago, Chicago, IL*; ³*Institute for Neuroscience, The University of Chicago, Chicago, IL*; ⁴*Institute for Biophysical Dynamics, The University of Chicago, Chicago, IL*; ⁵*Prizker School*

for Molecular Engineering, The University of Chicago, Chicago, IL

- TOG pm 02:50 **Optimization of HX-MS Workflow for Membrane Protein Melibiose Transporter MelB**; Yugi Shi¹; Hariharan Parameswaran²; Lan Guan²; Rosa Viner¹; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Department of Cell Physiology and Molecular Biophysics, Texas Tech University Health Sciences Center, Lubbock, TX*
- TOG pm 03:10 **Distinguishing Isomeric Disaccharides with In-electrospray Ionization Hydrogen/Deuterium Exchange-Mass Spectrometry (in-ESI HDX-MS)**; Ana V. Quintero¹; O. Tara Liyanage¹; Elyssia S. Gallagher¹; ¹*Baylor University, Waco, TX*
- TOG pm 03:30 **Transient structural dynamics during allosteric activation and inhibition of glycogen phosphorylase from non-equilibrium millisecond HDX-MS**; Monika Kish¹; Dylan P Ivory¹; Jonathan J Phillips¹; ¹*Living Systems Institute, University of Exeter, Exeter, United Kingdom*
- TOG pm 03:50 **Protein thermal depletion (PTD) coupled with long gradient sub-zero temperature UPLC-HDX-MS for elucidation of protein-ligand interactions in cell lysates**; Oliver Wu¹; Mulin Fang¹; Kellye A. Cupp-Sutton¹; Si Wu¹; ¹*University of Oklahoma, Norman, OK*
- TOG pm 04:10 **Selective protein capture under HDX-MS quench conditions for probing complex biological systems**; Dietmar Hammerschmid¹; Anthony Keeble²; Polina Heatley¹; Mark Howarth²; Eamonn Reading¹; ¹*Department of Chemistry, King's College London, London, United Kingdom*; ²*Department of Pharmacology, University of Cambridge, Cambridge, United Kingdom*

TOH pm: Clinical Analysis: Applications General Assembly C

Session Chair: Russell Grant (LabCorp)

- TOH pm 02:30 **Mass Spectrometry for the Underserved: A Chemical Signal Amplification Strategy for Asymptomatic Malaria Detection**; Abraham Kwame Badu-Tawiah¹; Ayesha Seth²; Muralikrishnan Girish²; Kingsley Badu³; ¹*The Ohio State University, Columbus, OH*; ²*Ohio State University, Columbus, OH*; ³*Kwame Nkrumah University of Science and Technology, Kumasi, Ghana*
- TOH pm 02:50 **Development of a Lead and Heavy Metal ICP-MS Assay from Quantitative Dried Blood Spots**; Donald H. Chace¹; Daniel Magiera²; NESTA Bortey-Sam³; Jerry Vockley⁴; ¹*Capitainer AB, Solna, Sweden*; ²*MMS Diagnostics, Warwick, RI*; ³*University of Pittsburgh, Pittsburgh, PA*; ⁴*University of Pittsburgh Medical Center, Pittsburgh, PA*
- TOH pm 03:10 **Tackling challenges in clinical plasma proteomics studies**; Jana Zecha¹; Junmin Wang²; Stefani N. Thomas³; Ventsislava A. Hristova¹; Sonja Hess¹; ¹*Dynamic Omics, Centre for Genomics Research (CGR), Discovery Sciences, Biopharmaceuticals R&D, Gaithersburg, MD*; ²*Data Sciences & Quantitative Biology, Discovery Sciences, Biopharmaceuticals R&D, AstraZeneca, Waltham, MA*; ³*Department of Laboratory Medicine and Pathology, University of Minnesota, Minneapolis, MN*
- TOH pm 03:30 **Targeted proteomics enables multiplex quantification of immunomodulatory and DNA mismatch repair proteins in FFPE tissue specimens**; Jeff Whiteaker¹; Lei Zhao¹; Uliana Voytovich¹; Jacob J. Kennedy¹; George Miles²; Galen Hostetter³; Chelsea Newton³; Scott Jewell²; Yongchao Dou²; Yuxing Liao²; Bing Zhang²; Andy

TUESDAY ORALS

Hoofnagle⁴; Shrabanti Chowdhury⁵; Pei Wang⁵; Amanda G. Paulovich¹; ¹*Fred Hutchinson Cancer Center, Seattle, WA*; ²*Baylor College of Medicine, Houston, TX*; ³*Van Andel Institute, Grand Rapids, MI*; ⁴*University of Washington, Seattle, WA*; ⁵*Icahn School of Medicine at Mount Sinai, New York, NY*

TOH pm 03:50 **Plasma Catecholamines by LC-MS/MS: Use of In-well Ion Pairing for Reverse Phase Retention and Interference Separation**; Stephen D Merrigan¹; Preejith P. Vachali¹; Elizabeth L. Frank²; ¹*ARUP Laboratories, Salt Lake City, UT*; ²*University of Utah, Salt Lake City, UT*

TOH pm 04:10 **Using robotic automation to advance standardisation and traceability in clinical diagnostics**; Tabatha Hambidge^{1,2}; Emily Whyte^{1,2}; Camilla Liscio³; Steven Corless¹; Patrick Sears²; Chris Hopley¹; ¹*LGC, Teddington, United Kingdom*; ²*University of Surrey, Guildford, United Kingdom*; ³*Element Materials Technology, Cambridge, United Kingdom*

WEDNESDAY ORALS

WOA am: Instrumentation: New Hybrid and Multimodal Approaches Hall B3

Session Chair: Benjamin Garcia (Washington University School of Medicine)

- WOA am 08:30 **Omnitrap-Orbitrap performance enhancement via unreduced data processing**; Anton N. Kozhinov¹; Konstantin O. Nagornov¹; Camille Garcia²; Tingting Fu²; Julia Chamot-Rooke²; Yury O. Tsybin¹; ¹Spectroswiss, Lausanne, Switzerland; ²Mass Spectrometry for Biology Unit, Institut Pasteur, Paris, France
- WOA am 08:50 **Implementation of 193nm UVPD on a trapped ion mobility TOF mass spectrometer for the structural characterization of peptides and proteins**; Jamie P Butalewicz¹; Edwin Escobar¹; Christopher A. Wootton²; Melvin A Park³; Erin H. Seeley¹; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX; ²Bruker Daltonik GmbH, Bremen, Germany; ³Bruker Daltonics, Billerica, MA
- WOA am 09:10 **Adding a cryogenic IR spectroscopic dimension to LC-MS**; Ali H. Abikhodri¹; Stephan Warnke¹; Ahmed Ben Faleh¹; Thomas Rizzo¹; ¹Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland
- WOA am 09:30 **Pushing Frontiers of High-throughput High-resolution Analysis: Orbitrap Technology Unites with a New Star**; Alexander Makarov¹; Christian Hock¹; Hamish Stewart¹; Dmitry Grinfeld¹; Anastassios Giannakopoulos¹; Johannes Petzoldt¹; Toby Shanley¹; Eduard Denisov¹; Amelia Peterson¹; Matthew Garland¹; Nicolaie Eugen Damoc¹; Martin Zeller¹; Tabiwang N. Arrey¹; Anna Pashkova¹; Andreas Kuehn¹; Matthias Biel¹; Arne Kreuzmann¹; Bernd Hagedorn¹; Immo Colonius¹; Adrian Schuetz¹; Arne Stefes¹; Ankit Dwivedi¹; Daniel Mourad¹; Max Hoek¹; Philipp Cochems¹; Alexander Kholomeev¹; Robert Ostermann¹; Gregor Quiring¹; Maximilian Ochmann¹; Sascha Moehring¹; Alexander Wagner¹; Andre Petker¹; Sebastian Kanngiesser¹; Michael Wiedemeyer¹; Wilko Balschun¹; Frank Czemper¹; Vlad Zabrouskov²; Daniel Hermanson²; Andreas Wieghaus¹; Jean-Jacques Dunyach²; ¹Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ²Thermo Fisher Scientific, San Jose, CA
- WOA am 09:50 **Increased Signal-to-Noise Ratio and Speed of FT-IM-MS Experiments Using Nonlinear Frequency Modulation**; Elvin R. Cabrera¹; Brian H. Clowers¹; ¹Washington State University Department of Chemistry, Pullman, WA
- WOA am 10:10 **Ambient soft-landing enables cryo-EM sample preparation and structural elucidation of native proteins in electrified droplets**; Jingjin Fan¹; Zi Yang^{2,3}; Xiao Fan^{2,3}; Hongwei Wang^{2,3}; Xiaoyu Zhou¹; Zheng Ouyang¹; ¹Tsinghua University, Department of Precision Instrument, Beijing, China; ²Tsinghua University, Beijing, China; ³Tsinghua-Peking University Joint Center for Life Sciences, Beijing, China

WOB am: Biotherapeutics: Characterization and Quantitation Ballroom A

Session Chair: Pavel V. Bondarenko (Amgen)

- WOB am 08:30 **High-Throughput Bioanalytical Analyses of Therapeutic Antibodies Using FAIMS Combined with the SampleStream Platform and Intact Protein Mass Spectrometry**; Rachel Liqing Shi¹; Michael A. Dillon¹; Philip D. Compton²; Christoph Spiess¹; Jonathan L. Josephs¹; John C. Tran¹; ¹Genentech Inc, South San Francisco, CA; ²Integrated Protein Technologies Inc., Carlsbad, CA

- WOB am 08:50 **Rapid Characterization of Antibodies via Automated Flow Injection Coupled with Online Microdroplet Reactions and Native-pH Mass Spectrometry**; Hao Chen¹; Harsha P. Gunawardena²; Yongling Ai¹; Jinshan Gao³; Richard N Zare⁴; ¹New Jersey Institute of Technology, Newark, NJ; ²Janssen Research & Development, Spring House, PA; ³Montclair State University, Montclair, NJ; ⁴Stanford University, Stanford, CA
- WOB am 09:10 **The Use of Mass Spectrometry in Therapeutic Protein Biologics License Applications: A Retrospective Review Revisited**; Jamie Mans¹; Mercy Oyugi²; Bethel Asmelash¹; Cynthia Sommers¹; Sarah Rogstad²; ¹US Food and Drug Administration, Saint Louis, MO; ²US Food and Drug Administration, Silver Spring, MD
- WOB am 09:30 **Host cell protein (HCP) profiling and quantitation in gene therapy products on a novel high-resolution accurate mass platform**; Josh Smith¹; Sara Carillo¹; Kristina Srzentic²; Tabiwang N. Arrey²; Anna Pashkova³; Kai Scheffler³; Kelly Broster⁴; Nicolaie Eugen Damoc²; Jonathan Bones^{1,5}; ¹The National Institute for Bioprocessing Research & Training, Mount Merrion, Ireland; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ³Thermo Fisher Scientific, Reinach, Switzerland; ⁴Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; ⁵University College Dublin, Belfield, Ireland
- WOB am 09:50 **Pulsed Mode Charge Detection Mass Spectrometry Allows Selective Analysis of Gene Therapy Products in Unpurified Samples**; Daniel Y. Botamanenko¹; Benjamin E. Draper¹; Martin F. Jarrold²; ¹Megadalon Solutions, Bloomington, IN; ²Indiana University Bloomington, Bloomington, IN
- WOB am 10:10 **Oligonucleotide Mapping via LC-UV-MS/MS to Enable Comprehensive Primary Structure Characterization of an mRNA Vaccine Against SARS-CoV-2**; Andrew William Dawdy¹; Brian C Gau¹; Leah Hanliu Wang¹; Carlos H Castaneda¹; Olga V Friese¹; Matthew S Thompson²; Thomas F Lerch¹; David J Cirelli²; Jason C Rouse²; ¹Pfizer, Chesterfield, MO; ²Pfizer, Inc., Andover, MA

WOC am: Drug Discovery and Development: Qualitative and Quantitative Analysis

Ballroom B

Session Chair: Veronica Laos (Eli Lilly & Co.)

- WOC am 08:30 **Multi-omic analysis reveals changes in cellular pathways following MARC1 knockdown in mouse models of NASH**; David Chow¹; Yuanjun Guo¹; Edward Lagory¹; Han-Yin Yang¹; Bradford Gibson¹; Matthew Rardin¹; ¹Amgen, Inc., South San Francisco, CA
- WOC am 08:50 **Deciphering Deubiquitinase Ubiquitin Signaling and Substrate Degradation by DIA-PASEF**; He Zhu¹; Guillaume Adelmant²; Indrajit Sahu²; Nouf Alharbi²; Ujwal Punyamurtula²; Scott B. Ficarro²; Sara J. Buhlage³; Jarrod A. Marto²; ¹Dana-Farber Cancer Institute, Boston, MA; ²Department of Cancer Biology, Department of Oncologic Pathology, Blais Proteomics Center, Dana-Farber Cancer Institute, Boston, MA; ³Department of Cancer Biology and the Linde Program in Cancer Chemical Biology, Dana-Farber Cancer Institute, Boston, Massachusetts
- WOC am 09:10 **Developing high-throughput screening MALDI-TOF MS cellular assays for drug discovery in non-alcoholic fatty liver disease**; Ruth H Walker¹; José Luis Marín-Rubio¹; Frank H. Büttner²; Matthias Trost¹; Maria Emilia Dueñas¹; ¹Biosciences Institute Faculty of Medical Sciences, Newcastle University, NE2 4HH, Newcastle Upon Tyne, United Kingdom;

WEDNESDAY ORALS

- WOC am 09:30 ²*Drug Discovery Sciences, Boehringer Ingelheim Pharma GmbH & Co. KG, Birkendorfer Str. 65, Biberach an der Riß, Germany*
Simultaneous In situ Pharmacological Profiling of Transcription Factors for Cancer Therapy; Lindsay K Pino¹; Andrea Gutierrez¹; Julia E Robbins¹; Carolyn Allen¹; Erin Broderick¹; Tonibelle Gatbonton-Schwager¹; Brian McEllin¹; Sebastian Paez¹; Yang Gao¹; William E Fondrie¹; Daniele Canzani¹; Alexander Federation¹; ¹*Talus Bioscience, Seattle, WA*
- WOC am 09:50 **Employing mass spectrometry and positional peptide patterns to probe for bioactive peptides;** Christian T Madsen¹; Jan C. Refsgaard¹; Felix G. Teufel¹; Sonny K. Kjærulff¹; Zhe Wang²; Guangjun Meng²; Carsten Jessen¹; Petteri Heljo¹; Qunfeng Jiang²; Xin Zhao²; Bo Wu²; Xueping Zhou²; Yang Tang²; Jacob F. Jeppesen¹; Christian D. Kelstrup¹; Stephen T. Buckley¹; Søren Tullin¹; Jan Nygaard-Jensen¹; Xiaoli Chen²; Fang Zhang²; Jesper V. Olsen³; Dan Han²; Mads Grønberg¹; Ulrik De Lichtenberg⁴; ¹*Novo Nordisk A/S, Måløv, Denmark*; ²*Novo Nordisk A/S, Beijing, China*; ³*NovoNordisk Center for Protein Research, København, Denmark*; ⁴*The Novo Nordisk Foundation, Hellerup, Denmark*
- WOC am 10:10 **Structural Elucidation in Drug metabolism and chemical degradation studies for molecules of any size and any high Resolution Acquisition modes;** Fabien Fontaine¹; Tatiana Radckenko¹; Paula Cifuentes¹; Albert Garriga¹; Xavier Pascual¹; Luca Moretoni²; Nadia Zara²; Ismael Zamora¹; ¹*Lead Molecular Design, S.L., Sant Cugat del Valles, Spain*; ²*Molecular Discovery, Elstree Borehamwood, United Kingdom*

WOD am: Artificial Intelligence in MS Instrumentation and Applications Ballroom C

Session Chair: Heather Desaire (University of Kansas)

- WOD am 08:30 **Development of a Predictive Multiple Reaction Monitoring (MRM) Model for High-throughput ADME Analyses Using Learning-to-Rank (LTR) Techniques;** Shivani Patel¹; Ramon Adalia²; Anthony Paiva¹; Ismael Zamora Rico²; Wilson Shou¹; Xianmei Cai¹; Tierni Kaufman³; ¹*Bristol Myers Squibb, Princeton, NJ*; ²*Lead Molecular Design, S.L., Sant Cugat del Valles, Spain*; ³*University of California, Berkeley, CA*
- WOD am 08:50 **“HODLING” When Ions Go “to the Moon”: a Tool that Should Make Us Rich But We’re Using for Mass Spectrometry;** Philip M Remes¹; Jesse Canterbury¹; William Barshop¹; Lillian Heil²; Cristina Jacob¹; Michael J. MacCoss²; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*University of Washington, Seattle, WA*
- WOD am 09:10 **Sequence-to-sequence translation from mass spectra to peptides with a transformer model;** Melih Yilmaz¹; William E Fondrie²; Wout Bittremieux³; Rowan Nelson¹; Varun Ananth¹; Sewoong Oh¹; William S Noble¹; ¹*University of Washington, Seattle, WA*; ²*Talus Bioscience, Seattle, WA*; ³*University of Antwerp, Antwerpen, Belgium*
- WOD am 09:30 **Improving Peptide Identification Rate by Machine Learning with Second-Ranked Peptide Spectrum Matches;** Johra Muhammad Moosa¹; Bin Ma^{1,2}; ¹*University of Waterloo, Waterloo, ON*; ²*Rapid Novor Inc., Kitchener, ON*
- WOD am 09:50 **Probabilistic modeling of peptide chromatography with Chronologer-NF provides novel insights into reverse phase chemistry;** Damien B Wilburn¹; Brian C. Searle²; ¹*Ohio State University, Columbus, OH*; ²*The Ohio State*

- WOD am 10:10 *University-Comprehensive Cancer Center, Columbus, OH*
Real-time Analysis and Classification of Aerosol Particles using Single-Particle Mass Spectrometry and Machine Learning; Heinrich Ruser¹; Guanzhong Wang¹; Julian Schade^{2,3}; Johannes Passig³; Thomas Adam^{2,4}; Ralf Zimmermann^{3,4}; ¹*University of Bundeswehr Munich, Institute for Applied Physics and Metrology, Neubiberg, Germany*; ²*University of Bundeswehr Munich, Faculty for Mechanical Engineering, Institute of Chemical and Environmental Engineering, Neubiberg, Germany*; ³*Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany*; ⁴*Joint Mass Spectrometry Center, Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, German Research Center for Environmental Health, Neuherberg, Germany*

WOE am: Industry: Trace Analysis, Quality Control, and Automation Room 332

Session Chair: Zhigang Hao (Colgate-Palmolive)

- WOE am 08:30 **Extractable profiling of a medical device component using an automated parallel extraction and evaporation system and the LC/MS multidetector approach;** Paulina Pinedo-Gonzalez¹; Dujuan Lu¹; Chongming Liu¹; Danny Hower¹; Aaron Lamb²; Jon Bardsley²; Min Du³; Sven Hackbusch⁴; ¹*SGS Health Science, Fairfield, NJ*; ²*Thermo Fisher Scientific, Manchester, United Kingdom*; ³*Thermo Fisher Scientific, Franklin, MA*; ⁴*Thermo Fisher Scientific, San Jose, CA*
- WOE am 08:50 **Comparative evaluation of the chemical preference in gender-stereotyped perfumes by GC-TOF MS;** Sunok Yoo¹; Hugh E. Jones¹; Mark P. Barrow¹; Diana Catalina Palacio Lozano¹; ¹*University of Warwick, Coventry, United Kingdom*
- WOE am 09:10 **Real-Time Measurement of Benzene in Aerosol Consumer Products using SIFT-MS;** Nicola Zenzola Heimbach¹; David Light¹; Kauri Kucera¹; Mara Dubnicka¹; Leslie Silva²; ¹*Valisure, LLC, New Haven, CT*; ²*Syft Technologies, Los Angeles, CA*
- WOE am 09:30 **Field-deployable LC-MS Platform for Environmental Monitoring Workflows: On-site Determination of Per, and Polyfluoroalkyl Substances (PFAS);** John Lam¹; Mohamed Hemida¹; Navneet Singh²; Matthew Askeland²; Pawel Kidon²; Fraser Smith¹; Andrew Gooley¹; ¹*Trajan Scientific and Medical, Ringwood, Australia*; ²*ADE Consulting Group, Williamstown North, Australia*
- WOE am 09:50 **A universal workflow for fully automated sample preparation in large-scale proteomics;** Luca Sandro Räss¹; Sandra Schaefer¹; Marco Tognetti¹; Roland Bruderer¹; Lukas Reiter¹; ¹*BiognoSYS, Schlieren, Switzerland*
- WOE am 10:10 **Enantiomeric Purity Analysis of Synthetic Peptide Therapeutics by Direct Chiral High-Performance Liquid Chromatography-Electrospray Ionization Tandem Mass Spectrometry;** Laura K. Muehlbauer¹; Mark A. Strega¹; Trent J. Oman¹; Donald S. Risley¹; Ankur Jalan¹; Zhirui Lian¹; ¹*Eli Lilly and Company, Indianapolis, IN*

WOF am: Lipidomics: New MS Technologies and Applications General Assembly A

Session Chair: Hee-Yong Kim (National Institute on Alcohol Abuse and Alcoholism)

- WOF am 08:30 **Exploring lipid landscape and unraveling isomers using SLIM based High Resolution Ion**

WEDNESDAY ORALS

- WOF am 08:50 **Mobility**; Komal Kedia¹; Rachel Harris²; Kim Ekroos³; Kevin P. Bateman⁴; ¹Merck, west point, PA; ²MOBILion Systems, Chadds Ford, PA; ³Lipidomics Consulting Ltd., Irisvikkvägen 31D 02230, Finland; ⁴Merck, West Point, PA
- WOF am 09:10 **Spatially and temporally probing distinctive phospholipid alteration in Alzheimer's disease mouse brain via high-resolution ion mobility-enabled sn-position resolved lipidomics**; Shuling Xu¹; Zhijun Zhu¹; Daniel G. Delafield¹; Michael J. Rigby¹; Luigi Puglielli¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- WOF am 09:30 **In-Situ Droplet-Based Tissue Derivatization for Lipid Isomer Characterization Using LESA**; Dallas P. Freitas¹; Xi Chen¹; Erin A. Hirtzel¹; Madison E. Edwards¹; Joochan Kim¹; Hongying Wang¹; Yuxiang Sun¹; Klaudia I. Kocurek¹; David Russell¹; Xin Yan¹; ¹Texas A&M, College Station, TX
- WOF am 09:50 **Microscopy-directed Imaging Mass Spectrometry for Rapid High Spatial Resolution Molecular Imaging of Glomeruli**; Allison B Esselman^{1,2}; Nathan Heath Patterson^{2,3}; Lukasz G Migas^{2,4}; Martin Dufresne^{2,3}; Katerina V Djambazova^{2,5}; Madeline E Colley^{2,3}; Mark P De Caestecker⁶; Raf Van De Plas^{2,3,4}; Jeffrey M Spraggins^{1,2,3,5}; ¹Department of Chemistry, Vanderbilt University, Nashville, TN; ²Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ⁵Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; ⁶Division of Nephrology, Department of Medicine, Vanderbilt University, Nashville, TN
- WOF am 09:50 **Decreasing Relapse in Esogastric Cancer by Improved Diagnostic with SpiderMass Technology**; Léa Ledoux¹; Yanis Zirem²; Florence Renaud³; Michel Salzet²; Isabelle Fournier²; ¹Laboratoire PRISM - Université de Lille, Villeneuve d'ascq, France; ²PRISM Inserm U1192 - University of Lille, Villeneuve D'ascq Cedex, France; ³UMR-S 1192, Lille, France
- WOF am 10:10 **Integrated morphometric and molecular classification of central nervous system cancers using a unified platform with picosecond infrared laser mass spectrometry**; Alexa Fiorante¹; Michael Woolman¹; David Munoz¹; Gelareh Zadeh¹; Sunit Das¹; Howard Ginsberg¹; Arash Zarrine-Afsar¹; ¹University of Toronto, Toronto, ON
- WOG am 09:10 **Deep Proteome Turnover in human iPSC-derived Neurons**; Ashley Frankenfield¹; Jiawei Ni¹; Jamison Shih¹; Noah Smeriglio¹; Ling Hao¹; ¹George Washington University, Washington, DC
- WOG am 09:30 **Aziridination-Based 2-Aminopyridine Isotopic (AAPI) Tag Enables Lipid Accurate Quantification with Isomer Resolving Power**; Shuli Tang¹; Syuan-Ting Kuo¹; Hongyuan Yang¹; Luchen Wuyang¹; Jiaxin Feng¹; Xin Yan¹; ¹Texas A&M University, College Station, TX
- WOG am 09:50 **Spatial Neutron-Encoded Stable Isotopic Labeling of Three-Dimensional Multicellular Spheroids**; Arbil Lopez¹; Nicole C. Beller¹; Amanda B Hummon¹; ¹The Ohio State University, Columbus, OH
- WOG am 10:10 **Design and application of a plate-based, proteome-wide reactive cysteine profiling platform using vastly reduced starting protein amounts**; Ka Yang¹; Qing Yu¹; Shane Lillis Dawson¹; Joao A. Paulo¹; Steven P. Gygi¹; ¹Harvard Medical School, Boston, MA
- WOH am: Fundamentals: Ion Activation and Dissociation (Honoring Jean Futrell)**
General Assembly C
 Session Chair: Dick Smith (Pacific Northwest National Lab)
- WOH am 08:30 **Celebrating Jean Futrell's Career as a Mass Spectrometry Pioneer**; Julia Laskin; *Purdue University, West Lafayette, IN*
- WOH am 08:50 **Charging mechanisms of macromolecules in droplet-based ionization methods by linking electrostatic properties of parent solution, microscopic and nanoscopic droplets**; Styliani Consta¹; Yiming Qin²; ¹University of Western Ontario, London; ²University of California, Irvine, Irvine, CA
- WOH am 09:10 **Spontaneous fission of aqueous nanodrops with diameters <50 nm: effects of nanodrop size on charge loss**; Matthew S McPartlan¹; Conner C. Harper¹; Emeline Hanozin¹; Evan R. Williams¹; ¹University of California, Berkeley, Berkeley, CA
- WOH am 09:30 **Investigation of capillary position on repeatability, reproducibility, and unintentional in-source ion activation for different nESI sources**; Samantha O Shepherd¹; Austin W Green²; Kenneth R Newton^{2,3}; Elizabeth S Resendiz⁴; Ruwan T Kurulugama⁵; James S Prell²; ¹University of Oregon, Eugene, OR; ²University of Oregon, Department of Chemistry and Biochemistry, Eugene, OR; ³e-MSion, Corvallis, OR; ⁴University of California, Irvine, Irvine, CA; ⁵Agilent Technologies, Santa Clara, CA
- WOH am 09:50 **Measuring the absolute energy differences between conformers of protonated GlyProGlyGly**; Brandon C. Stevenson¹; Shannon Raab²; David E. Clemmer²; Peter B. Armentrout¹; ¹University of Utah, Salt Lake City, UT; ²Indiana University Bloomington, Bloomington, IN
- WOH am 10:10 **Differential labelling and mass spectrometry coupled with 473 nm photo-dissociation analysis for relative quantification of cysteine oxidation in proteins**; Marion Girod¹; Jean-Valery Guillaubez¹; Jérôme Lemoine¹; ¹University of Lyon, Villeurbanne, France
- WOG am: Stable Isotope Labeling: Applications**
General Assembly B
 Session Chair: Feixia Chu (University of New Hampshire)
- WOG am 08:30 **A novel strategy for the systematic analysis of protein degradation identifies direct targets of molecular glue degraders**; Marco Jochem¹; Anna Schrempf²; Lina-Marie Wagner¹; Georg Winter²; Jeroen Kriegsveld¹; ¹German Cancer Research Center (DKFZ), Heidelberg, Germany; ²CeMM Research Center for Molecular Medicine, Vienna, Austria
- WOG am 08:50 **Chiral Pair Isobaric Labeling Strategy for Multiplexed Absolute Quantitation (CHRISTMAS) Revealed Alteration of Enantiomeric DL-Amino Acids in Alzheimer's Disease Progression**; Zhijun Zhu¹; Shuling Xu¹; Zicong Wang¹; Daniel G. Delafield¹; Michael J. Rigby¹; Gaoyuan Lu¹; Ting-Jia Gu¹; Peng-Kai Liu¹; Min Ma¹; Luigi Puglielli¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI

WEDNESDAY ORALS

WOA pm: Instrumentation: Detection of High-Mass Analytes Hall B3

Session Chair: Nina Morgner (Goethe Universität Frankfurt)

- WOA pm 02:30 **Side by Side Comparison of Orbitrap Direct Mass Technology and Charge Detection Mass Spectrometry**; Martin Jarrold¹; *Indiana University, Chemistry Department, Bloomington, IN*
- WOA pm 02:50 **Benefits of ultra-long transients in Orbitrap based charge-detection mass spectrometry**; Evolène Deslignière¹; Victor Yin¹; Amber Rolland¹; Eduard Ebberink¹; Arjan Barendregt¹; Tobias P. Wörner²; Konstantin Nagornov³; Anton Kozhinov³; Kyle L. Fort²; Yury O. Tsybin³; Alexander A. Makarov²; Albert J.R. Heck¹; ¹*Utrecht University, Utrecht, Netherlands*; ²*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*; ³*Spectroswiss, Lausanne, Switzerland*
- WOA pm 03:10 **To 200k m/z and beyond: native electron-capture charge reduction resolves heterogeneous signals in large biopharmaceutical analytes, a new Orbitrap record**; Kyle I.P. Le Huray^{1,2}; Tobias P. Woerner²; Maria Reinhardt-Szyba²; Kyle L. Fort²; Frank Sobott¹; Alexander A. Makarov²; ¹*University of Leeds, Leeds, United Kingdom*; ²*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*
- WOA pm 03:30 **Differential Ion Mobility Separations of Intact Antibodies and Complexes: Taking FAIMS of Macromolecules Toward the MegaDalton Range**; Tobias P Wörner¹; Hayden A Thurman²; Alexander A Makarov¹; Alexandre A Shvartsburg²; ¹*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*; ²*Wichita State University, Wichita, KS*
- WOA pm 03:50 **Protein complex heterogeneity and structure revealed by native mass spectrometry with electron capture charge reduction and surface induced dissociation**; Jared B. Shaw¹; Sophie R. Harvey²; Chen Du³; Vicki H Wysocki^{2,3}; ¹*e-MSion, Corvallis, OR*; ²*Resource for Native Mass Spectrometry-Guided Structural Biology, The Ohio State University, Columbus, OH*; ³*Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH*
- WOA pm 04:10 **Large and in Charge: Rapid Analysis of 300+ MDa Nanoparticles and Biomolecules Using High-Throughput, Filter-less Charge Detection Mass Spectrometry (CDMS)**; Conner C Harper¹; Zachary M. Miller¹; Matthew S. McPartlan¹; Jacob S. Jordan¹; Evan R. Williams¹; ¹*University of California, Berkeley, Berkeley, CA*

WOB pm: Biomarkers: Qualitative Analysis Ballroom A

Session Chair: Carlito Lebrilla (University of California, Davis)

- WOB pm 02:30 **Deepest profiling of healthy human tissues to date sheds light on expressed proteins**; Sandra Schär¹; Marco Tognetti¹; Roland Bruderer²; Lukas Reiter²; ¹*Biognosys AG, Schlieren, Switzerland*; ²*Biognosys AG, Schlieren, Switzerland*
- WOB pm 02:50 **A meta-omics workflow to generate a novel host and microbial biomarker panel for early detection of ovarian cancer**; Subina Mehta¹; Kristin Boylan¹; Ashley J. Petersen¹; Amy P.N. Skubitz¹; Pratik D Jagtap¹; Timothy J Griffin¹; ¹*University of Minnesota, Minneapolis, MN*
- WOB pm 03:10 **Placeholder for talk in WOB pm**; Jennifer Anne Watson; *ASMS Office, Santa Fe, NM*
- WOB pm 03:30 **Pushing DIA proteomics analyses of neat plasma to 1000 proteins/h**; Ines Metatla¹; Kévin Roger¹; Cerina Chhuon¹; Anne Jamet²; Maria Leite De Moraes²; Manuel Chapelle³; Pierre-Olivier Schmit³; Chiara Guerrera¹; ¹*Proteomics Platform Necker, Paris, France*; ²*INSERM U1151 - CNRS*

¹*UMR 8253, Institut Necker-Enfants Malades, Paris, France*; ³*Bruker Daltonique S.A., Wissembourg, France*

- WOB pm 03:50 **Metabolomics in Nuclear Emergencies: Application of Small Molecule Assays for Complex Exposures to Ionizing Radiation**; Evan Pannkuk¹; Evagelia Laiakis¹; Guy Garty²; Brian Ponnaiya²; Xuefeng Wu²; Igor Shuryak²; Shanaz Ghandhi²; Sally Amundson²; David Brenner²; Albert Fornace, Jr.¹; ¹*Georgetown University, Washington Dc, DC*; ²*Columbia University, New York, New York, United States, New York*
- WOB pm 04:10 **Development of Senescence-Associated Monocyte Proteome Signatures in Human Clinical Studies**; Reema Banarjee¹; Bradley Olinger¹; Dimitrios Tsiatsipatis¹; Anjana Ram¹; Theodoe Nyunt¹; Ceereena Ubaida-Mohien¹; Gulzar Daya¹; Zhongsheng Peng¹; Myriam Gorospe¹; Luigi Ferrucci¹; Keenan Walker¹; Nathan Basisty¹; ¹*National Institute on Aging, Baltimore, MD*

WOC pm: Metabolomics: New Technologies and Applications Ballroom B

Session Chair: Facundo Fernandez (Georgia Institute of Technology)

- WOC pm 02:30 **Current practices in LC-MS untargeted metabolomics: a scoping review on the use of pooled quality control samples**; Corey D Broeckling¹; Richard Beger²; Leo L Cheng³; Raquel Cumeras⁴; Daniel J Cuthbertson⁵; Surendra Dasari⁶; Clay W Davis⁷; Warwick B Dunn⁸; Anne M Evans⁹; Álvaro Fernández-Ochoa¹⁰; Kelli D Goodman⁹; Helen Gika¹¹; Royston Goodacre⁸; Goncalo J Gouveia¹²; Hsu Ping-Ching¹³; Jennifer A Kriwan¹⁴; Dritan Kodra¹¹; Julia Kuligowski¹⁵; Lan S Renny¹⁶; María Eugenia Monge¹⁷; Jonathan D Mosley¹⁸; Sindhu Nair¹⁹; Nichole Reisdorph²⁰; Stacy D Sherrod²¹; Georgios Theodoridis¹¹; Candice Z Ulmer Holland²²; Dajana Vuckovic²³; Bo Zhang²⁴; ¹*Colorado State University, Fort Collins, CO*; ²*National Center for Toxicological Research, Jefferson, AR*; ³*Harvard Medical School, Boston, MA*; ⁴*Institut d'Investigació Sanitària Pere Virgili, Tarragona, Spain*; ⁵*Agilent Technologies, Santa Clara, CA*; ⁶*Mayo Clinic, Rochester, MN*; ⁷*National Institute of Standards and Technology, Charleston, SC*; ⁸*University of Liverpool, Liverpool, United Kingdom*; ⁹*Metabolon, Morrisville, NC*; ¹⁰*University of Granada, Granada, Spain*; ¹¹*Aristotle University of Thessaloniki, Thessaloniki, Greece*; ¹²*National Institute of Standards and Technology, Rockville, MD*; ¹³*University of Arkansas for Medical Sciences, Little Rock, AR*; ¹⁴*Max Delbrück Center, Berlin, Germany*; ¹⁵*Health Research Institute La Fe, Valencia, Afghanistan*; ¹⁶*Arkansas Children's Nutrition Center, Little Rock, AR*; ¹⁷*Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Buenos Aires, Argentina*; ¹⁸*Environmental Protection Agency, Athens, GA*; ¹⁹*University of Alberta, Edmonton, AB*; ²⁰*University of Colorado Anschutz, Denver, CO*; ²¹*Vanderbilt University, Nashville, TN*; ²²*USDA-FSIS, Athens, GA*; ²³*Concordia University, Montreal, Qc*; ²⁴*Olaris, Framingham, MA*
- WOC pm 02:50 **Development of a High-Coverage and Quantitative Metabolomics Assay for Targeted Analysis of Multiple Pathways**; Shuang Zhao¹; Liang Li¹; ¹*The Metabolomics Innovation Centre (TMIC) - University of Alberta, Edmonton, AB*
- WOC pm 03:10 **Mass spectrometry-related tools expand the underappreciated diversity of bile acids and their biological implications**; Helena Mannocho Russo¹; Ipsita Mohanty¹; Yasin El Abiead¹; Joshua V Schweer¹; Robin Schmid¹; Simone Zuffa¹; Wout

WEDNESDAY ORALS

Bittremieux²; Felipe Vasquez-Castro¹; Andrew D Patterson³; Dionicio Siegel¹; Lee Hagey¹; Mingxun Wang⁴; Allegra T Aron⁵; Pieter C Dorrestein¹; ¹University of California San Diego, San Diego, CA; ²University of Antwerp, Antwerpen, Belgium; ³Pennsylvania State University, State College, University Park, PA 16803; ⁴University of California Riverside, Riverside, CA; ⁵University of Denver, Denver, CO

WOC pm 03:30 **Integrating quantification of low abundant targets into nontargeted LC-MS/MS screening using Simultaneous Quantitation and Discovery (SQUAD);** Elys Rodriguez¹; Uri Keshet¹; Bashar Amer²; Sunandini Yelda³; Brandon Bills³; Tong Shen¹; Susan Bird³; Oliver Fiehn¹; ¹University of California Davis, Davis, CA; ²Thermo Fisher Scientific, San Jose, California; ³ThermoFisher Scientific, San Jose, CA

WOC pm 03:50 **Introducing Owlstone's Breath Biopsy VOC Atlas: identification of breath VOCs with TD-GC-Orbitrap high resolution accurate mass spectrometry;** Shane Swann¹; Wisenave Arulvasan¹; Ace Hatch¹; Julia Greenwood¹; Dominic Roberts²; Billy Boyle¹; Max Allsworth¹; ¹Owlstone Medical, Cambridge, United Kingdom; ²Thermo Fisher Scientific, Manchester, United Kingdom

WOC pm 04:10 **Development of a multi-omic approach for microorganism identifications;** Jana M Carpenter¹; Kingsley Bimpeh¹; Hannah Hynds¹; Kelly Hines¹; ¹University of Georgia, Athens, GA

WOD pm: Challenges in MS Analysis of Complex Mixtures Ballroom C

Session Chair: Christian Rolando (Université de Lille)

WOD pm 02:30 **FT-ICR MS Reveals Molecular Composition of Dissolved Organic Matter from Non-terrestrial Materials;** Joseph Frye-Jones^{1,2}; Martha L Chacón-Patiño²; Ryan P Rodgers^{1,2}; Alan G Marshall^{1,2}; ¹Florida State University, Tallahassee, FL; ²National High Magnetic Field Laboratory, Tallahassee, FL

WOD pm 02:50 **Enhancing Hydrophilic Metabolite Detection and Quantifiability via Derivatization-Assisted Sample Preparation and Dispersive Liquid-Liquid Microextraction (DLLME) Techniques;** Olga L Riusech¹; Lingjun Li¹; ¹University of Wisconsin, Madison, WI

WOD pm 03:10 **Structural Elucidation of Lipopolysaccharides using Field Asymmetric Ion Mobility Spectrometry and Kendrick Mass Defect Plots;** Abanoub Mikhael¹; Darryl Hardie¹; Derek Smith¹; Helena Petrosova¹; Robert K Ernst²; David R Goodlett^{1,3}; ¹University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; ²University of Maryland, Baltimore, MD; ³University of Victoria, Victoria, BC

WOD pm 03:30 **Comprehensive impurities profiling in synthetic oligonucleotides by high-resolution mass spectrometry intact mass data processing;** A M Abdullah¹; Cynthia Sommers¹; Jason Rodriguez¹; Deyi Zhang²; Darby Kozak²; Kui Yang¹; ¹US Food and Drug Administration, Saint Louis, MO; ²US Food and Drug Administration, Silver Spring, MD

WOD pm 03:50 **Advancing to ultra-high throughput for broad plasma proteome profiling using a novel high-resolution accurate mass platform;** Qin Fu¹; Tabiawang N. Arrey²; Niveda Sundararaman¹; Eugen Damoc²; Yue Xuan²; Jennifer E. Van Eyk¹; ¹Cedars Sinai Medical Center, Los Angeles, CA; ²Thermo Fisher Scientific, Bremen, Germany

WOD pm 04:10 **Polymer Analysis on a High-Resolution Quadrupole-Multi Reflecting Time-of-Flight Mass Spectrometer;** Bryan C. Katzenmeyer¹; Dale A. Cooper-Shepherd²; Martin E. Palmer³; ¹Waters

Corporation, Milford, MA; ²Waters Corporation, Wilmslow, United Kingdom; ³Waters, Wilmslow, United Kingdom

WOE pm: GC/MS: Instrumentation and Applications Room 332

Session Chair: Jean-Francois Focant (University of Liege)

WOE pm 02:30 **The Expected and Unexpected Multiple Benefits of GC-MS with Cold EI;** Aviv Amirav¹; Benny Neumark¹; Oneg Elkabets¹; Alex Yakovchuk¹; ¹Tel-Aviv University, Tel-Aviv, Israel

WOE pm 02:50 **Enhancing the Coverage and Quality of Spectra of per- and polyfluoroalkyl Substances in a Comprehensive Electron Ionization Mass Spectral Library;** Yufang Zheng¹; Edward Erisman¹; Tytus D. Mak¹; Weihua Ji¹; William E. Wallace¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD

WOE pm 03:10 **Unequivocal identification and trace level determination of microplastics present in Mediterranean beaches by pyrolysis-GC/MS with F-Search tools;** Lucia H.M.L.M. Santos^{1,2}; Sara Insa^{1,2}; Marta Arxé^{1,2}; Gianluigi Buttiglieri^{1,2}; Sara Rodríguez-Mozaz^{1,2}; Damia Barcelo^{1,2,3}; ¹Catalan Institute for Water Research (ICRA), Girona, Spain; ²University of Girona, Girona, Spain; ³Institute of Environmental Assessment and Water Research - Spanish Council for Scientific Research (IDAEA-CSIC), Barcelona, Spain

WOE pm 03:30 **Structural library of oxidized lipid-derived volatiles and its application to breath biomarker discovery;** Yuta Matsuoka¹; Yuki Sugiura²; ¹Kyoto university, Kyoto, Japan; ²Kyoto University, Kyoto, Japan

WOE pm 03:50 **Exploring Mosquito Olfactory Preferences with Whole Body Volatilomics;** Stephanie Rankin-Turner¹; Diego Giraldo¹; Conor McMeniman¹; ¹Johns Hopkins Bloomberg School of Public Health, Baltimore, MD

WOE pm 04:10 **Identification of Different Hydrocarbons in Aviation Fuels by Using Two-Dimensional Gas chromatography/Methane Chemical Ionization Time-of-Flight Mass Spectrometry;** Caroline E. R. Rowell¹; Jacob D. Guthrie¹; Michael E. Peretich²; Gozdem Kilaz¹; Hilka I. Kenttämaa¹; ¹Purdue University, West Lafayette, IN; ²Naval Air Warfare Center Aircraft Division, Patuxent River, MD

WOF pm: Quantitative Proteomics in Systems Biology General Assembly A

Session Chair: Kerriann Backus (UCLA)

WOF pm 02:30 **High-throughput sample multiplexing-based targeted pathway proteomics with real-time analytics reveals the impact of genetic variation on protein expression;** Steven P Gygi¹; Qing Yu¹; Xinyue Liu¹; Mark Keller²; Tian Zhang¹; Steven Shuken¹; Ernst Schmid¹; Edward L Huttlin¹; Devin Schweppe³; Alan D Attie⁴; Joao A Paulo¹; ¹Harvard Medical School, Boston, MA; ²University of Wisconsin-Madison, Madison, WI; ³University of Washington, Seattle, WA; ⁴University of Wisconsin, Madison, WI

WOF pm 02:50 **Multiplexed quantification of endogenous membrane protein complexes in native mass spectrometry;** Jack L Bennett^{1,2,3}; Corinne A Lutomski^{1,2}; Tarick J El-Baba^{1,2}; Sophie AS Lawrence^{1,2}; Joshua D Hinkle⁴; Christopher Mullen⁵; John EP Syka⁵; Carol V Robinson^{1,2}; ¹Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; ²Department of Chemistry, University of Oxford, Oxford, United Kingdom; ³School of Chemistry, UNSW Sydney, Sydney,

WEDNESDAY ORALS

- WOF pm 03:10 *Australia*; ⁴*Thermo Fisher Scientific, San Jose, CA*; ⁵*ThermoFisher Scientific, San Jose, CA*
A multidimensional proteomic atlas of replicative aging in budding yeast; Mario Leuter¹; Joe Armstrong¹; Anja R Ollodart¹; Kyle N Hess¹; Michael Muir²; Ricard A Rodriguez-Mias¹; Matt Kaerberlein²; Maitreya Dunham¹; Judit Villén¹; ¹*Department of Genome Sciences, University of Washington, Seattle, WA*; ²*Department of Laboratory Medicine and Pathology, University of Washington, Seattle, WA*
- WOF pm 03:30 **Mapping communication dynamics between physically interacting cells using HySiC**; Kelly E Stecker¹; Sofia Ibanez-Molero²; Tatiana M. Shamorkina¹; Rosa Viner³; Daniel S. Peeper²; Maarten A.F.M. Altelar¹; ¹*Utrecht University, Utrecht, Netherlands*; ²*Netherlands Cancer Institute, Amsterdam, Netherlands*; ³*Thermo Fisher Scientific, San Jose, CA*
- WOF pm 03:50 **Evaluation of the Relative Quantitative Performance Using Tandem Mass Tags on a New High-Resolution Accurate Mass Platform**; Martin Zeller¹; Jenny Ho²; Amirmansoor Hakimi³; Maowei Dou⁴; Ryan Bomgarden⁴; Rosa Viner³; Bernd Hagedorn¹; Ankit Dwivedi¹; Nicolaie Eugen Damoc¹; ¹*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*; ²*Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*; ³*Thermo Fisher Scientific, San Jose, CA*; ⁴*Thermo Fisher Scientific, Rockford, IL*
- WOF pm 04:10 **The day after the drug: understanding persister-derived cells to uncover the mechanisms underlying non-genetic cancer resistance**; Bianca J Kuhn¹; Natalie Clark¹; D. R. Mani¹; Adi Goldstein²; Yaara Oren²; Steven A Carr¹; Namrata D Udeshi¹; ¹*Broad Institute of MIT and Harvard, Cambridge, MA*; ²*Tel Aviv University, Tel Aviv, Israel*

WOG pm: Fundamentals: Reactions of Gaseous and Solvated Ions

General Assembly B

Session Chair: David Foreman (Merck)

- WOG pm 02:30 **Evidence of the Role of the 5f-Orbitals in An+ Reactivity in ICP-MS/MS Reactions with CO₂ and NO_x**; Richard Cox¹; Amanda D. French¹; Kali M. Melby¹; Micah Prange¹; Niri Govind¹; ¹*Pacific Northwest National Laboratory, Richland, WA*
- WOG pm 02:50 **Structural differentiation of denatured ubiquitin conformers via gas-phase ion/ion cross-linking reactions coupled with infrared multiphoton dissociation**; Woo-Young Kang¹; Arup Mondal¹; Julia R. Bonney¹; Alberto Perez¹; Boone M. Prentice¹; ¹*University of Florida, Gainesville, FL*
- WOG pm 03:10 **Variable Temperature H/D Exchange and Ion-Neutral Clustering using FT-IM-MS to Probe Solvation Dynamics**; Haley M Schramm¹; Tomoya Tamadate²; Christopher J Hogan²; Brian H Clowers¹; ¹*Washington State University Department of Chemistry, Pullman, WA*; ²*University of Minnesota, Minneapolis, MN*
- WOG pm 03:30 **Theta-capillary-based interfacial microreactor for reaction acceleration and intermediate capture**; Madison E Edwards¹; Erin A. Hirtzel²; Dallas Freitas²; Annesha Sengupta²; Joohan Kim²; Xin Yan²; ¹*Texas A&M Chemistry, College Station, TX*; ²*Texas A&M, College Station, TX*
- WOG pm 03:50 **Methanol-Catalysed Isomerism of Aryl-Amine Protomers**; Boris Ucur¹; Oisín J Shiels¹; Alan T Maccarone¹; Shane R. Ellis^{1,2}; Stephen J Blanksby²; Adam J Trevitt¹; ¹*University of Wollongong, School of Chemistry, Wollongong, Australia*; ²*Illawarra Health and Medical Research*

- WOG pm 04:10 *Institute, Wollongong, Australia*; ³*Central Analytical Research Facility, Institute for Future Environments, Brisbane, Australia*
A New Mechanism for Water Splitting from Gas-Phase Fragmentation of Water Clusters with Holmium Nitrate Complexes; Jungsoo Kim; *Idaho National Laboratory, Idaho Falls, ID*

WOH pm: Environmental: Non-Target Analysis and Emerging Contaminants

General Assembly C

Session Chair: Imma Ferrer (University of Colorado Boulder)

- WOH pm 02:30 **Identifying the Toxins of Harmful Algal Blooms with High Resolution Mass Spectrometry**; Logan C Krajewski¹; Kirsten A Cottrill²; Willam A Bragg¹; Brady R Cunningham¹; Noelani R Boise³; Kristin D Victry³; Dana L Woodruff³; Karen L Wahi³; David S Wunschel³; Rudolph C Johnson¹; Elizabeth I Hamelin¹; ¹*Centers for Disease Control and Prevention, Atlanta, GA*; ²*Battelle Memorial Insitute at the Centers for Disease Control and Prevention, Atlanta, GA*; ³*Pacific Northwest National Laboratory, Richland, WA*
- WOH pm 02:50 **Library Matching in Real-Time for Guided Data-Dependent HRAM Analysis of Unknown PFAS**; Brandon Bills¹; Sunandini Yedla¹; Ed George¹; Juan Sanchez¹; Tim Stratton¹; Ralf Tautenhahn¹; Vlad Zabrouskov¹; ¹*Thermo Fisher Scientific, San Jose, California*
- WOH pm 03:10 **Non-targeted identification of chemical markers to authenticate honey botanical origin using LC-QTOF-MS**; Lei Tian¹; Shaghig Bilamjian¹; Tarun Anumol²; Daniel Cuthbertson²; Stéphane Bayen¹; ¹*McGill University, Ste-Anne-de-Belleuve, QC*; ²*Agilent Technologies, Santa Clara, CA*
- WOH pm 03:30 **Uncovering the Fate of High Latitude Oil Spills: Non-target LC-Orbitrap Analysis of Hydrocarbon Oxidation Products**; Maxwell L. Harsha¹; Danielle E. Verna²; Zachary C. Redman³; Josh Wesolowski³; Angélique Fouche³; David C. Podgorski^{1,3}; Patrick L Tomco^{1,3}; ¹*University of New Orleans, New Orleans, LA*; ²*Prince William Sound Regional Citizens' Advisory Council, Valdez, AK*; ³*University of Alaska Anchorage, Anchorage, AK*
- WOH pm 03:50 **Tissue distributions and metabolism of known and novel PFASs in mice dosed with a complex aqueous film-forming foam (AFFF) mixture**; David Dukes¹; Carrie A McDonough²; ¹*Stony Brook University, Stony Brook, NY*; ²*Carnegie Mellon University, Pittsburgh, PA*
- WOH pm 04:10 **Toward wider accessibility of a non-targeted standard/quality control mixture for more reliable method development/assessments**; Christine M. Fisher¹; Ann M. Knolhoff¹; ¹*FDA Center for Food Safety, College Park, MD*

THURSDAY ORALS

ThOA am: Instrumentation: Ambient Ionization and Applications Hall B3

Session Chair: Hao Chen (New Jersey Institute of Technology)

- ThOA am 08:30 **Melting needles in haystacks: Fast laser heating coupled to solution-phase separations for measuring protein thermal stabilities from complex matrices;** [Jacob S. Jordan](#)¹; Evan R. Williams¹; ¹University of California, Berkeley, Berkeley, CA
- ThOA am 08:50 **A monolithic microfluidic probe for ambient mass spectrometry imaging of biological tissues;** [Lixue Jiang](#)¹; Matthias Polack²; Manxi Yang¹; Xiangtang Li³; Detlev Belder²; Julia Laskin³; ¹Purdue University, West Lafayette, IN; ²Leipzig University, Leipzig, Germany; ³Purdue University, Lafayette, IN
- ThOA am 09:10 **Towards Molecular Digital Twins for Oncology Surgery with Real-Time SpiderMass Mass Spectrometry Imaging;** Nina Ogrinc¹; Paul Chaillou¹; Lea Ledoux¹; Michel Salzet¹; [Isabelle Fournier](#)¹; ¹PRISM Inserm U1192 - University of Lille, Villeneuve D'ascq Cedex, France
- ThOA am 09:30 **Advances in Venturi Easy Ambient Sonic-Spray Ionization;** [Luan Felipe C Oliveira](#)¹; David U. Tega²; Alessandra Sussulini²; Xin Yan³; Lane A. Baker³; ¹Texas A&M, College Station, TX; ²University of Campinas, Campinas, Brazil; ³Texas A&M Chemistry, College Station, TX
- ThOA am 09:50 **Temperature-Controllable Spark Probe Ionization for Multi-dimensional Mass Spectrometer Analysis;** Ningxi Li¹; [Xinwei Liu](#)¹; Zhijun Cai¹; Zongyao Zhang¹; Jiexun Bu²; Simin Cheng¹; Xiaoxiao Ma¹; Wenpeng Zhang¹; Xiaoyu Zhou¹; Zheng Ouyang¹; ¹Tsinghua University, Beijing, China; ²PURSPEC Technologies (Beijing) Inc., Beijing, China
- ThOA am 10:10 **Next-generation Portable Ambient Ionization Mass Spectrometer with Integrated 2D MS/MS Capabilities;** [Dalton Snyder](#)¹; Leonard Rorrer¹; Mitch Wells¹; Megan Guetzloff¹; Jane Likens¹; Nicole Huckaby¹; Harman Casey¹; Kevin Rosenbaum¹; Brandon Reese¹; Austin Stieglitz¹; Anthony Eshleman¹; Luther Collins¹; Brett Atkinson¹; ¹Teledyne FLIR, West Lafayette, IN

ThOB am: Glycopeptides, Glycoproteins, and Glycomics Ballroom A

Session Chair: Cheng Lin (Boston University)

- ThOB am 08:30 **Glycosite mapping and structural dynamics of TIM family immune checkpoints enabled by mucinase SmE;** Joann Chongsaritsinsuk¹; Alexandra D. Steigmeyer¹; Keira E. Mahoney¹; Mia A. Rosenfeld²; Taryn M. Lucas¹; Deniz Ince¹; Fiona L. Kearns²; Alexandria Battison¹; Michael J. Ferracane³; Rommie E. Amaro²; [Stacy A. Malaker](#)¹; ¹Yale University, New Haven, CT; ²University of California San Diego, San Diego, CA; ³University of Redlands, Redlands, CA
- ThOB am 08:50 **Benefits of dual ion routing multipoles for glycoproteomics;** [Nicholas M. Riley](#)^{1,2}; Jingjing Huang³; David Bergen³; William D. Barshop³; John E.P. Syka³; Jesse D. Canterbury³; Vlad Zabrouskov³; Graeme C. McAllister³; Christopher Mullen³; ¹Stanford University, Stanford, CA; ²University of Washington, Seattle, WA; ³Thermo Fisher Scientific, San Jose, CA
- ThOB am 09:10 **Characterization of multi-glycosylated proteins by combining O-glycoprotease IMPa and 193 nm ultraviolet photodissociation;** [Amanda Helms](#)¹; Edwin Escobar^{1,2}; Saulius Vainauskas²; Christopher H. Taron²; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX; ²New England Biolabs, Ipswich, MA

- ThOB am 09:30 **Discovery of unusual high-mannose N-glycans by new multi-stage tandem mass spectrometry;** Chia Yen Liew^{1,2,3}; Hong-Sheng Luo^{1,4}; Ting-Yi Yang^{1,4}; An-Ti Hung^{1,5}; Bryan John Abel Magoling^{1,6}; Charles Pin-Kuang Lai^{1,6}; [Chi-Kung Ni](#)⁷; ¹IAMS, Academia Sinica, Taipei, Taiwan; ²International Graduate Program of Science and Technology (MST), National Taiwan University, Taipei, Taiwan; ³Molecular Science and Technology (MST), Taiwan International Graduate Program (TIGP), Taipei, Taiwan; ⁴Department of Chemistry, National Taiwan Normal University, Taipei, Taiwan; ⁵Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan; ⁶Chemical Biology and Molecular Biophysics Program, Taiwan International Graduate Program, Academia Sinica, Taipei, Taiwan; ⁷Academia Sinica, Taipei, Taiwan

- ThOB am 09:50 **Mass-defect peak fingerprints embedded by 6-plex mdSUGAR tag labeling guide targeted high-resolution mass spectrometry for ultra-sensitive glycomics;** [Min Ma](#)¹; Miyang Li²; Yinlong Zhu^{3,4}; Yingyi Zhao⁵; Feixuan Wu¹; Zicong Wang¹; Yu Feng¹; Hung-Yu Chiang⁶; Cheng Chang^{3,7}; Lingjun Li^{1,8}; ¹School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ²Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ³State Key Laboratory of Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences (Beijing), Beijing Institute of Lifeomics, Beijing, China; ⁴Chongqing Key Laboratory on Big Data for Bio Intelligence, Chongqing University of Posts and Telecommunications, Chongqing, China; ⁵State Key Laboratory of Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences (Beijing), Beijing Institute of Lifeomics, Beijing, China; ⁶Biophysics Program, University of Wisconsin-Madison, Madison, WI; ⁷Research Unit of Proteomics Driven Cancer Precision Medicine, Chinese Academy of Medical Sciences, Beijing, China; ⁸Department of Chemistry, University of Wisconsin - Madison, Madison, WI

- ThOB am 10:10 **Expanding the MSFragger Glyco Toolkit with O-Pair Localization of O-Glycopeptides in FragPipe;** [Daniel Polasky](#)¹; Lei Lu²; Fengchao Yu¹; Guo Ci Teo¹; Michael R. Shortreed³; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI; ²University of California San Francisco, San Francisco, CA; ³University of Wisconsin-Madison, Madison, WI

ThOC am: Metabolomics: Untargeted Profiling Ballroom B

Session Chair: Kirsten Overdahl (National Institute of Environmental Health Sciences (NIEHS))

- ThOC am 08:30 **QA/QC for Untargeted Metabolomics in a Large Core Lab: Current Best Practices and Innovative Strategies;** [Uri Keshet](#)¹; Gert Wohlgemuth¹; Fanzhou Kong¹; Yuanyue Li¹; Diego Pedrosa¹; Oliver Fiehn¹; ¹UC Davis, Davis, CA
- ThOC am 08:50 **Untargeted metabolomics by high-resolution mass spectrometry as an enhanced tool for food quality classification;** [Angela Di Capua](#)¹; Maria Assunta Acquavia¹; Carmine Gaeta²; Patrizia Iannece²; Rosanna Ciriello¹; Filomena Lelario¹; Carmen Tesoro¹; Roberto Rubino³; Giuliana Bianco¹; ¹Università degli Studi della Basilicata, Dipartimento di Scienze, via dell'Ateneo Lucano 10, 85100, Potenza, Italy; ²Università Degli Studi di Salerno, Dipartimento di Chimica e Biologia, Via Giovanni Paolo II 132,84084, Fisciano (SA), Italy; ³ANFoSC - Via San Leonardo 62/A, 84131, Salerno, Italy

THURSDAY ORALS

- ThOC am 09:10 **Dual column chromatography improves non-targeted analysis coverage when assessing rhizosphere chemical communication;** Alexandra A Bennett¹; Çağla Gökem Eroğlu²; Teresa Steininger-Mairinger¹; Markus Puschenreiter³; Aurélie Gfeller²; Judith Wirth²; Stephan Hann¹; ¹University of Natural Resources and Life Sciences, Vienna, Department of Chemistry, Institute of Analytical Chemistry, Vienna, Austria; ²Agroscope, Department of Plant-Production Systems, Herbology in Field Crops Research Group, Nyon, Switzerland; ³University of Natural Resources and Life Sciences, Vienna, Department of Forest- and Soil Sciences, Institute of Soil Research, Vienna, Austria
- ThOC am 09:30 **Real-Time Breath Analysis Towards a Healthy Human Breath Baseline;** Zachary J. Sasiene¹; Erick S. Lebrun¹; Eric G. Schaller²; Phillip M. Mach¹; Robert M. Taylor²; Trevor G. Glaros¹; Justin T. Baca²; Ethan M. McBride¹; ¹Los Alamos National Laboratory, Los Alamos, NM; ²University of New Mexico, Department of Chemical and Biological Engineering, Albuquerque, NM
- ThOC am 09:50 **Untargeted metabolomics reveals severity biomarkers for Type 2 Diabetes mellitus and related complications in the Indian population;** Pramod P. Wangikar^{1,2}; Sneha A Rana¹; Vivek Mishra²; Prajval Nakrani²; Bhushan Burkul²; Rakesh Kumar Sahay³; Lakshman Kumar³; ¹Indian Institute of Technology Bombay, Mumbai, India; ²Clarity Bio Systems India Pvt Ltd, Pune, India; ³osmania medical college, Hyderabad, India
- ThOC am 10:10 **Molecular network-based optimization of annotations in GC-MS;** Alexander Semenov¹; Vladimir Boginski²; Alexey Melnik³; Alexander Aksenov³; ¹University of Florida, Gainesville, FL; ²University of Central Florida, Orlando, FL; ³University of Connecticut, Storrs, CT
- ThOD am 09:10 **Rapid single-shot proteomics using narrow window DIA on a novel high-resolution accurate mass (HRAM) platform;** Ana Martinez Del Val¹; Ulises H. Guzmán¹; Zilu Ye¹; Florian Harking¹; Ole Østergaard¹; Anna Pashkova²; Tabiwang N. Arrey²; Hamish Stewart²; Yue Xuan²; Nicolaie Eugen Damoc²; Jesper V. Olsen¹; ¹Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- ThOD am 09:30 **A protein turnover atlas across 15 mouse tissues established by DIA and TMT;** Wenxue Li¹; Ka Yang²; Abhijit Dasgupta²; Junmin Peng²; Yansheng Liu¹; ¹Yale Cancer Biology Institute, West Haven, CT; ²St. Jude Children's research hospital, Memphis, TN
- ThOD am 09:50 **Extracellular Matrix Proteomics of Human Lungs Enabled by a Photocleavable Surfactant and diaPASEF;** Elizabeth F. Bayne¹; Yanlong Zhu^{2,3}; Kevin M. Buck¹; Melissa R. Pergande^{2,3}; Vanessa Morales-Tirado⁴; Yupeng He⁵; Yu Tian⁶; Ying Ge^{1,2,3}; ¹Department of Chemistry, University of Wisconsin - Madison, Madison, WI; ²Department of Cell and Regenerative Biology, University of Wisconsin - Madison, Madison, WI; ³Human Proteomics Program, University of Wisconsin - Madison, Madison, WI; ⁴Discovery Immunology, Pharmacology and Pathology, AbbVie Bioresearch Center, Worcester, MA; ⁵Discovery Immunology, Pharmacology and Pathology, AbbVie Inc., North Chicago, IL; ⁶DMPK-BA, AbbVie Bioresearch Center, Worcester, MA
- ThOD am 10:10 **Parkin Activator, PR-364 Protects Cardiomyocytes Post-Heart Attack: Increased Mitochondrial Function and Translational Reprogramming;** Lizhuo Ai¹; Aleksandr Stotland¹; Simion Kreimer¹; Matthew Ayres¹; Juliana De Freitas Germano¹; Chengqun Huang¹; Tauseef Butt²; Suresh Kumar²; Roberta Gottlieb¹; Jennifer Van Eyk¹; ¹Cedars-Sinai Medical Center, Los Angeles, CA; ²Progenra Inc, Malvern, PA
- ThOD am: Data-Independent Acquisition and Multiplexing: Proteomics**
Ballroom C
 Session Chair: Birgit Schilling (Buck Institute)
- ThOD am 08:30 **Over 5000 proteins quantified in plasma using DIA-PASEF analysis of nanoparticle protein corona on TIMS-TOF HT Mass Spectrometer;** Hasmik Keshishian¹; Michael W. Burgess¹; Sebastian Vaca²; Joseph Allen¹; Elizabeth D. Lightbody³; Irene M. Ghobrial³; D. R. Mani¹; Michael A. Gillette^{1,4}; Matt Willetts⁵; Steven A Carr¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²Bruker Scientific, San Jose, CA; ³Dana Farber Cancer Institute, Boston, MA; ⁴Massachusetts General Hospital, Boston, MA; ⁵Bruker Scientific, LLC, Billerica, MA
- ThOD am 08:50 **Multiplex-DIA enhances single-cell proteomic depth via a reference channel;** Marvin Thielert¹; Corazon Ericka Mae Itang²; Constantin Ammar²; Florian A. Rosenberger²; Isabell Bludau²; Patricia Skowronek²; Maria Wahle²; Wen-Feng Zeng²; Xie-Xuan Zhou²; Andreas-David Brunner^{2,3}; Sabrina Richter^{4,5}; Fabian J Theis^{4,5}; Martin Steger^{2,6}; Matthias Mann^{2,7}; ¹Max Planck Institute of Biochemistry, Martinsried, Munich, Germany; ²Max-Planck-Institute for Biochemistry, Martinsried, Germany; ³Boehringer Ingelheim Pharma, Biberach, Germany; ⁴Helmholtz Zentrum München – German Research Center for Environmental Health, Neuherberg, Germany; ⁵Technical University of Munich, Freising, Germany; ⁶NEOsphere Biotechnologies GmbH, Planegg, Germany; ⁷Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark
- ThOE am: Fundamentals Beyond Mass Analysis: Structural Characterization of Isomers**
Room 332
 Session Chair: Gabe Nagy (University of Utah)
- ThOE am 08:30 **Everything but the kitchen sink: Combining IMS-IMS, cryogenic IR spectroscopy, and MS to tackle the isomer problem in oligosaccharide analysis;** Ali H. Abikhodr¹; Stephan Warnke¹; Ahmed Ben Faleh¹; Vasylyatsyna¹; Thomas Rizzo¹; ¹Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
- ThOE am 08:50 **Beyond Mass Spectrometry: Negative Ion Photoelectron Spectra of 1-, 2-, and 3-Cyanoanthracene Radical Anions and the Thermochemistry of Cyanoanthracene Isomers;** Wilson Gichuhi¹; Aidan J. Usher¹; Kie T. Workman¹; ¹Tennessee Tech University, Cookeville, TN
- ThOE am 09:10 **Identification and relative quantification of fatty acid double bond positional isomers in biological tissues using gas-phase charge inversion ion/ion reactions;** Julia R. Bonney¹; Boone M. Prentice¹; ¹University of Florida, Gainesville, FL
- ThOE am 09:30 **Tracking Isomerizations in High-Energy Adenine and 9-Methyladenine Cation Radicals by UV-Vis Photodissociation Action Spectroscopy and Cyclic Ion Mobility;** Václav Zima¹; Jiahao Wan¹; Mikuláš Vlček²; Josef Cvačka²; František Tureček¹; ¹University of Washington, Seattle, WA; ²Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic

THURSDAY ORALS

- ThOE am 09:50 **A universal photosensitizer for isomer-resolved mass spectrometry imaging of lipids using singlet oxygen reaction;** Sara Amer¹; Daisy M Unishuay Vila^{1,2}; Mushfeqa Iqfath¹; Julia Laskin¹; ¹Purdue University, West Lafayette, Indiana; ²University of Pennsylvania, Philadelphia, PA
- ThOE am 10:10 **Characterization of sialylated N-glycopeptide isomers on reversed phase LC-ECD mass spectrometry;** Suya Liu¹; Zoe Zhang¹; Pavel Ryumin¹; Takashi Baba¹; ¹AB SCIEX, Concord, ON

**ThOF am: Protein-Ligand and Protein-Protein Interactions
General Assembly A**
Session Chair: Kallol Gupta (Yale University)

- ThOF am 08:30 **BioPlex 3D: Predicting Structures for Protein-protein Interactions across the Human Interactome;** Edward L. Huttlin¹; Julian Mintseris¹; Roger Vargas¹; Laura Pontano Vaites¹; Tyrone Lee¹; Sanjukta Guha Thakurta¹; Lana D'Addieco¹; Fana Gebreab¹; Emily Hill¹; Daniel Linnehan¹; David Vanderwall¹; Brandon Gassaway¹; Sherry Liu¹; Joao A Paulo¹; Qing Yu¹; Jose Navarrete-Perea¹; Josh Pan²; David P Nusinow³; Tess C Branon³; Donald S Kirkpatrick³; Ludwig Geistlinger¹; Robert Gentleman¹; J. Wade Harper¹; Steve Gygi¹; ¹Harvard Medical School, Boston, MA; ²Broad Institute of MIT and Harvard, Cambridge, MA; ³Interline Therapeutics, Brisbane, CA
- ThOF am 08:50 **Characterizing the interactions between the HIV-1 capsid protein and small molecule ligands using native mass spectrometry;** Sophie Harvey^{1,2}; William M McFadden³; Bruce E Torbett^{4,5}; Stefan G Sarafianos^{3,6}; Vicki H Wysocki^{1,2}; ¹Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; ²Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; ³Center for ViroSciences and Cure, Laboratory of Biochemical Pharmacology, Department of Pediatrics, Emory University School of Medicine, Atlanta, Georgia; ⁴Department of Pediatrics, University of Washington School of Medicine, Seattle, WA; ⁵Center for Immunity and Immunotherapies, Seattle Children's Research Institute, Seattle, WA; ⁶Children's Healthcare of Atlanta, Atlanta, Georgia
- ThOF am 09:10 **Native Top-Down Mass Spectrometry Probes Membrane Protein Structures and Lipid Binding Sites;** Jessie Le¹; Pascal Egea²; Mark Arbing²; Rachel R. Ogorzalek Loo²; Joseph A. Loo²; ¹University of California - Los Angeles, Los Angeles, CA; ²University of California, Los Angeles, Los Angeles, CA
- ThOF am 09:30 **Native Mass Spectrometry Captures Protein Interactions Responsible for Inflammatory Cell Death;** Jonathan T S Hopper¹; Kleitos Sokratous¹; Antonio Biasutto¹; Emma Norgate¹; James Lloyd²; Karolina Gherbi¹; Idir Liko¹; Neil Oldham²; ¹OMass Therapeutics, Oxford, United Kingdom; ²University of Nottingham, Nottingham, United Kingdom
- ThOF am 09:50 **RAPID ANALYSIS OF PROTEIN-PROTEIN INTERACTIONS USING A NOVEL HIGH-RESOLUTION ACCURATE MASS PLATFORM;** Lia Serrano¹; Danielle Swaney^{2,3,4,5}; Tabiwang N. Arrey⁶; Trenton M. Peters-Clarke¹; Noah M Lancaster¹; Anna Pashkova⁶; Evgenia Shishkova¹; Michael S. Westphall¹; Christian Hock⁶; Nicolai Eugen Damoc⁶; Vlad Zabrouskov⁶; Joshua J. Coon^{1,7}; ¹University of Wisconsin-Madison, Madison, WI; ²QBI COVID-19 Research Group (QCRG), San Francisco, CA; ³Quantitative Biosciences Institute (QBI), University of California San Francisco, San Francisco, CA; ⁴J. David Gladstone Institutes, San Francisco, CA; ⁵Department of Cellular and

Molecular Pharmacology, University of California San Francisco, San Francisco, CA; ⁶Thermo Fisher Scientific, Bremen, Germany; ⁷Morgridge Institute for Research, Madison, WI

- ThOF am 10:10 **Benchmarks and protocols for top-down mass spectrometry of native proteins and complexes: A consortium-based study;** Tanja Habeck¹; Kyle A. Brown²; Benjamin Des Soye³; Carter Lantz⁴; Mowei Zhou⁵; Novera Alam⁶; Md Amin Hossain⁶; Wonhyeuk Jung⁴; James E. Keener⁷; Michael Volny⁸; Jesse W. Wilson⁵; Yujia Ying⁹; Jeffrey N. Agar⁶; Paul O. Danis¹⁰; Ying Ge²; Neil L. Kelleher³; Huilin Li⁹; Joseph A. Loo⁴; Michael T. Marty⁷; Ljiljana Paša-Tolić⁵; Wendy Sandoval⁸; Frederik Lermyte¹; ¹Technical University of Darmstadt, Darmstadt, Germany; ²University of Wisconsin-Madison, Madison, WI; ³Northwestern University, Evanston, IL; ⁴University of California, Los Angeles, Los Angeles, CA; ⁵Pacific Northwest National Laboratory, Richland, WA; ⁶Northeastern University, Boston, MA; ⁷University of Arizona, Tucson, AZ; ⁸Genentech Inc, South San Francisco, CA; ⁹Sun Yat-sen University, Guangzhou, China; ¹⁰Consortium for Top-Down Proteomics, Cambridge, MA

**ThOG am: Microbes and the Microbiome
General Assembly B**
Session Chair: Tian (Autumn) Qiu (Michigan State University)

- ThOG am 08:30 **Untargeted mass spectrometry-based metabolomics reveals responses to high fiber whole-food diets and microbiome composition in mice;** Jacob J. Haffner^{1,2}; Yi Sun^{3,4}; Daniela Betancurt Anzola⁵; Evan R. Hutchison³; Eugenio I. Vivas³; Robert L. Kerby³; Nsoua H. Diaba⁶; Camil Gosmanov⁶; Alejandro Reyes Muñoz⁵; Federico E. Rey³; Laura-Isobel McCall^{2,6,7}; ¹University of Oklahoma, Department of Anthropology, Norman, OK; ²University of Oklahoma, Laboratories of Molecular Anthropology and Microbiome Research, Norman, OK; ³University of Wisconsin-Madison, Department of Bacteriology, Madison, WI; ⁴Northwest A&F University, College of Food Science and Engineering, Xianyang, China; ⁵Universidad de los Andes, Departamento de Ciencias Biológicas, Bogotá, Colombia; ⁶University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; ⁷University of Oklahoma, Department of Microbiology and Plant Biology, Norman, OK
- ThOG am 08:50 **MINNO: A new platform for interpreting complex microbial metabolomics data;** Stephanie L Bishop¹; Ayush Mandwal¹; Mehdi Mohammadi¹; Thomas Rydzak¹; Ryan A Groves¹; Mildred Castellanos¹; George Chaconas¹; Joern Davidsen¹; Ian A Lewis¹; ¹University of Calgary, Calgary, AB
- ThOG am 09:10 **Evaluating the benefit of dia-PASEF approaches and sample-specific database strategies for metaproteomics of very complex microbiomes;** Thibaut Dumas¹; Olivier Pible¹; Guylaine Miotello¹; Kristina Marx²; Pierre-Olivier Schmit^{2,3}; Jean Armengaud¹; ¹CEA-Marcoule - Laboratory «Innovative technologies for Detection and Diagnostics», Bagnols-sur-Cèze, France; ²Bruker Daltonics GmbH & Co.KG, Bremen, Germany; ³Bruker France S.A., Wissembourg, France
- ThOG am 09:30 **On-chip multi-modal imaging of soil biogeochemical processes using Synthetic Soil Habitats;** Arunima Bhattacharjee¹; Jocelyn Richardson²; Dušan Veličković¹; Gregory Vandergrift¹; Christopher Anderton¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Stanford University, Palo Alto, CA

THURSDAY ORALS

- ThOG am 09:50 **Reliable and high-resolution 3D MS imaging of complex biofilms;** Yuting Shen^{1,2}; Kangning Ren^{1,2}; Zongwei Cai^{1,2}; ¹*State Key Laboratory of Environmental and Biological Analysis, Hong Kong, China*; ²*Department of Chemistry, Hong Kong Baptist University, Hong Kong, China*
- ThOG am 10:10 **Mapping Cellular Organization and Molecular Distributions in *S. aureus* Abscesses;** Jacqueline M. Van Ardenne^{1,2}; Lukasz G Migas³; Madeline E Colley^{4,5}; Martin Dufresne^{2,5}; Jeffrey A Freiberg⁶; Valeria M Reyes Ruiz⁶; Andy Weiss⁶; Katerina V Djambazova^{2,7}; Katherine N Gbison-Corley⁶; Raf Van De Plas^{2,3,5,7}; Eric P Skaar⁶; Jeffrey M Spraggins^{1,2,5,7}; 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*Mass Spectrometry Research Center, 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 Cell and Developmental Biology, Vanderbilt University, Nashville, TN*

ThOH am: Nucleic Acids and Oligonucleotides General Assembly C

Session Chair: Jennifer Lippens (Janssen Pharmaceutica NV)

- ThOH am 08:30 **Identification of critical impurities in starting materials for oligonucleotide therapeutics by derivatization with reactive chromophores;** Rajeswari Lakshmanan¹; Andrew Rodriguez¹; Phil Olsen¹; Dennis Rhodes¹; Claus Rentel¹; ¹*Ionis Pharmaceuticals, Inc., Carlsbad, CA*
- ThOH am 08:50 **Sequence mapping and rapid quality control analysis of mRNA therapeutics using mass spectrometry;** Emma N Welbourne¹; Caroline Evans¹; Christina Vanhinsbergh¹; Mark Dickman¹; ¹*University of Sheffield, Sheffield, United Kingdom*
- ThOH am 09:10 **LC-HRMS-based Multi-Attribute Method for Oligonucleotides (MAMO);** Kui Yang¹; A M Abdullah¹; Md Rabiul Islam¹; Nnenna E Dieke¹; Cynthia Sommers¹; Jason Rodriguez¹; Deyi Zhang²; Darby Kozak²; David Keire¹; ¹*US FDA, St. Louis, MO*; ²*US Food and Drug Administration, Silver Spring, MD*
- ThOH am 09:30 **Characterisation and sequencing of modified large mRNA products by nanoflow liquid chromatography coupled to high resolution mass spectrometry;** Craig Jakes¹; Maikel Gaitkoski^{1,2}; Felipe Guapo¹; Silvia Millan Martin¹; Sara Carillo¹; Jonathan Bones^{1,2}; ¹*National Institute of Bioprocessing Research and Training, Dublin, Ireland*; ²*School of Chemical and Bioprocess Engineering, University College Dublin, Dublin, Ireland*
- ThOH am 09:50 **Ion Trap Collision-induced Dissociation as a Probe of G-quadruplex Formation;** Nicole M Brundridge¹; Jonathan Dickerhoff¹; Danzhou Yang¹; Scott A McLuckey¹; ¹*Purdue University, Dept. of Chemistry, West Lafayette, IN*
- ThOH am 10:10 **Complete sequencing of large modified peptide-nucleic acids using MALDI TOF MS/MS;** Daniil G Ivanov¹; John J Thomas²; Dani M Stoltzfus²; Igor A Kaltashov¹; ¹*University of Massachusetts Amherst, Amherst, MA*; ²*NeuBase Therapeutics, Pittsburgh, PA*

THURSDAY ORALS

ThOA pm: Instrumentation: Innovative Separation Approaches Coupled to MS Hall B3

Session Chair: Alexander Ivanov (Northeastern University)

- ThOA pm 02:30 **Open Tubular Solid Phase Extraction Columns Enable Simple and Robust Nanoflow Liquid Chromatography for Single-Cell Proteomics;** Kei Webber¹; Siqui Huang¹; Thy Truong¹; Xiaofeng Xie¹; Ryan Kelly¹; ¹Brigham Young University, Provo, UT
- ThOA pm 02:50 **Photoinitiator-Integrated Mobile Phases for Protein Disulfide Mapping By LC/MS2 : Intact versus Bottom-up Approach and pH Effect;** Shu-Hui Chen¹; Chin-Ming Kuo¹; Fung-Yu Chen¹; ¹National Cheng Kung University, Tainan, Taiwan
- ThOA pm 03:10 **Exploring Charge Detection Mass Spectrometry on Liquid Chromatography Time Scales;** Lisa Strasser¹; Florian Fuessl¹; Tomos E. Morgan¹; Felipe Guapo¹; Sara Carillo¹; Jonathan Bones^{1,2}; ¹NIBRT, Dublin, Ireland; ²School of Chemical and Bioprocess Engineering, University College Dublin, Dublin, Ireland
- ThOA pm 03:30 **Unifying the Multi-Omics World with Microchip Capillary Electrophoresis: Discovering Secrets in Six Dimensions from One Drop of Dried Blood;** J. Will Thompson^{1,2}; J. Scott Mellors¹; Youwei Chen²; Timothy McMahon²; Matthew W Foster²; ¹908 Devices Inc, Carrboro, NC; ²Duke University Medical Center, Durham, NC
- ThOA pm 03:50 **Enhanced Sensitivity for Low-Load Proteomics Orbitrap Workflows Using Ion Fractionation with Structures for Lossless Ion Manipulation;** Daniel Debord¹; Liulin Deng¹; Brian Adamson²; Alan McKenzie-Coe¹; Kyle L. Fort³; Tobias Woerner³; Oliver M Bernhardt⁴; Roland Bruderer⁴; Tejas Gandhi⁴; Lukas Reiter⁴; Eloy R Wouters²; Jean-Jacques Dunyach²; Alexander Makarov³; ¹MOBILion Systems, Chadds Ford, PA; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ⁴Biognosys AG, Schlieren, Switzerland
- ThOA pm 04:10 **Rapid and accurate quantitation of therapeutic drugs by coupling capillary electrophoresis with miniature mass spectrometry system;** Xiao Chen¹; Junhan Wu¹; Yikun Liu¹; Wenpeng Zhang¹; Zheng Ouyang¹; ¹Tsinghua University, Beijing, China

ThOB pm: Biotherapeutics: Proteins, Antibodies, and Antibody/Drug Conjugates Ballroom A

Session Chair: Andrew Mahan (Janssen Pharmaceutical)

- ThOB pm 02:30 **Discovery and Characterization of an Acid-Labile Crosslinker in Antibody High Molecular Weight Species Using Mass Spectrometry Methods;** Gaoyuan Liu¹; Yuetian Yan¹; Shunhai Wang¹; Ning Li¹; ¹Regeneron Pharmaceuticals Inc., Tarrytown, NY
- ThOB pm 02:50 **Mass spectrometry-based process analytical technology used for rapid online and at-line process and product characterization in biopharmaceuticals;** David Naoki Powers¹; Nicole Azer¹; Aron Gyorgypal²; Erica Berilla¹; Casey Kohnhorst¹; ¹FDA, Silver Spring, MD; ²Rutgers University, New Brunswick, NJ
- ThOB pm 03:10 **Ion Mobility-Mass Spectrometry and Collision Induced Unfolding Rapidly Classify Human IgG2 Cysteine to Serine Exchange Variants;** Rosendo C. Villafuerte-Vega¹; Hayden Fisher²; Isabel Elliott²; Mark S Cragg²; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI; ²University of Southampton, Southampton, United Kingdom
- ThOB pm 03:30 **Internal Fragments Enhance Middle-down Mass Spectrometry Structural Characterization of**

Monoclonal Antibodies and Antibody-drug

Conjugates; Bengian Wei¹; Carter Lantz¹; Rachel R. Ogorzalek Loo¹; Iain D. G. Campuzano²; Joseph A. Loo¹; ¹UCLA, Los Angeles, CA; ²Amgen, Thousand Oaks, CA

- ThOB pm 03:50 **Antibody structural dynamics investigated by covalent labelling and structure-sensitive fragmentation;** Melissa Ann Coxhead¹; Dale A. Cooper-Shepherd²; Romina Hofele³; Paul Devine⁴; Nicholas J. Bond⁴; Frank Sobott¹; ¹University of Leeds, Leeds, United Kingdom; ²Waters Corporation, Stamford Ave, Altrincham Road, Wilmslow, United Kingdom; ³Analytical Sciences, BioPharmaceutical Development, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, Maryland; ⁴Analytical Sciences, BioPharmaceutical Development, BioPharmaceuticals R&D, AstraZeneca, Cambridge, United Kingdom
- ThOB pm 04:10 **Glycosylation-dependent stability and aggregation behavior of an immuno-regulatory protein complex revealed by native ion mobility mass spectrometry;** Philipp Bittner¹; Felix Kuhne²; Dietmar Reusch²; Renato Zenobi¹; ¹ETH Zurich, Zurich, Switzerland; ²Roche Diagnostics GmbH, Pharma Technical Development, Penzberg, Germany

ThOC pm: Imaging: Pharmaceuticals, Metabolites, Lipids, and Glycans Ballroom B

Session Chair: Michelle Reyzer (Vanderbilt University)

- ThOC pm 02:30 **Mass spectrometry imaging DESI-TQMS for brain biodistribution evaluation of new radiopharmaceuticals;** Antoine Lefèvre¹; Emmanuelle Claude²; Sylvie Bodard¹; Sylvie Chalon¹; Julie Busson¹; Johnny Vercoillie¹; Freddy Drouy³; Laurent Galigne¹; Patrick Emond^{1,4}; ¹University Tours, INSERM, iBrain, UMR 1253, Tours, France; ²Waters Corporation, Wilmslow, United Kingdom; ³Waters Corporation, Guyancourt, France; ⁴CHRU Tours, Serv Med Nucl Vitro, Tours, France
- ThOC pm 02:50 **Age-related N-glycan changes in human skin biopsies identified by MALDI FTICR imaging.;** Samuele Zoratto^{1,2}; Mirjam Balbis^{1,3}; Christopher Kremsehner^{2,4}; Sandra Forestier^{2,5}; Gaëlle Gendronneau^{2,5}; Florian Gruber^{2,4}; Martina Marchetti-Deschmann^{1,2}; ¹TU Wien, Vienna, Austria; ²Christian Doppler Laboratory for Multimodal Imaging of Aging and Senescence - SKINMAGINE, Vienna, Austria; ³MS Proteomics Research Group, Research Centre for Natural Sciences, Budapest, Hungary; ⁴Medical University of Vienna, Department of Dermatology, Vienna, Austria; ⁵Chanel PB, Pantin, France
- ThOC pm 03:10 **Advancing spatial N-glycomics with MALDI-MSI to reveal molecular signatures of degenerative glomeruli in diabetic kidney disease;** Dušan Veličković¹; Jeffrey Hodgkin²; Theodore Alexandrov³; Kumar Sharma⁴; Christopher Anderton¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²University of Michigan Ann-Arbor, Ann Arbor, MI; ³EMBL, Heidelberg, Germany; ⁴University of Texas Health San Antonio, San Antonio, TX
- ThOC pm 03:30 **Steatoda nobilis Female and Male: A Comparative Study Including Full Body MALDI-FT-ICR Imaging and Deep Venom Characterization.;** Damien Redureau¹; John Dunbar²; Antoine Fort³; Virginie Bertrand¹; Raphaël La Rocca¹; Christopher Kune¹; Sophie Rappe¹; Ronan Sulpice³; Edwin De Pauw¹; Michel Dugon²; Loïc Quinton¹; ¹MS-Lab, MOLSys Research Unit,

THURSDAY ORALS

University of Liège, Liège, Belgium; ²Venom Systems Lab - School of Natural Sciences - University of Galway, Galway, Ireland; ³Plant Systems Biology Lab, Plant and AgriBiosciences Research Centre, School of Natural Sciences, Ryan Institute, National University of Ireland Galway, Galway, Ireland

ThOC pm 03:50 **MALDI IMS identifies changes in lipids and metabolites in rat brains following arsenic exposure;** E. Ellen Jones¹; Dustyn Barnette¹; Laura Schnackenberg¹; Richard Beger¹; Andrew Shen¹; Timothy Flanigan¹; ¹FDA/NCTR, Jefferson, AR

ThOC pm 04:10 **Single-cell lipidomics enabled by high-throughput mass spectrometry imaging at subcellular resolution;** Hua Zhang¹; Yuan Liu¹; Xudong Shi²; Penghsuan Huang³; Haiyan Lu¹; Andrew J. Schneider^{4,5}; Luigi Puglielli^{4,5}; Nathan V. Welham²; Lingjun Li^{1,3}; ¹School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ²Department of Surgery, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WISCONSIN; ³Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ⁴Department of Medicine, University of Wisconsin-Madison, Madison, WISCONSIN; ⁵Waisman Center, University of Wisconsin-Madison, Madison, WISCONSIN

ThOD pm: Fundamentals: Ion Structures and Energetics Ballroom C

Session Chair: Bela Paizs (Rosalind Franklin Institute)

ThOD pm 02:30 **Deprotonated Glycan Dissociation Chemistry;** Ola Bataineh¹; Lauren Schultz¹; Benjamin J. Bythell²; ¹Ohio University, Athens, OH; ²Ohio University, Athens, OH

ThOD pm 02:50 **Taming Conformational Heterogeneity of N-Methylated Macrocyclic Peptides on an Ion Race Track;** Thanh D Do¹; Hernando J. Olivos²; Miranda N. Limbach¹; Damilola S. Oluwatoba¹; Jonathan K. Martens³; Jos Oomens³; ¹University of Tennessee, Knoxville, Knoxville, TN; ²Waters Corporation, Milford, MA; ³HFML FELIX, Radboud University, Netherlands

ThOD pm 03:10 **Conformational heterogeneity of top-down fragment ions analyzed by tandem-trapped ion mobility spectrometry/mass spectrometry (tTIMS/MS);** Thais Pedrete¹; Tyler C Cropley¹; Fanny C Liu¹; Jusung Lee¹; Christian Bleiholder¹; ¹Florida State University, Tallahassee, FL

ThOD pm 03:30 **Simulations of Surface-Induced Dissociation Mass Spectrometry of a Protein Dimer Essential for Hearing;** Zachary D Smith¹; Yu-Fu Lin¹; Dalton Snyder^{1,2}; Vicki H Wysocki¹; Marcos Sotomayor¹; ¹Ohio State University, Columbus, OH; ²Teledyne FLIR, West Lafayette, IN

ThOD pm 03:50 **Investigation of Transient Species through Metal Clusters of Triphenylphosphine Chalcogenides with Group I Metals;** Brittany Hodges¹; Jungsoo Kim¹; Christopher A. Zarzana¹; ¹Idaho National Laboratory, Idaho Falls, ID

ThOD pm 04:10 **Coulomb explosion molecular imaging: direct characterization of complex structures through multivariate analysis;** Michael Burt¹; Louis Minion²; James Somper¹; ¹University of Oxford, Oxford, United Kingdom; ²Imperial College London, London, United Kingdom

ThOE pm: Environmental: Innovative Approaches and Instrumentation Room 332

Session Chair: Nathan Dalleska (California Institute of Technology)

ThOE pm 02:30 **2-Nitrofluoroglucinol as an Effective Matrix for Quantitative MALDI MS and Imaging of Fungicide Pyrimethanil in Strawberries;** Heather McDonald¹; Qi Li²; Md Ashaduzzaman²; Chao Zhao²; Shanlin Pan²; Gregory J. Szulczewski²; Qiaoli Liang²; ¹University of West Alabama, Livingston, AL; ²University of Alabama, Tuscaloosa, AL

ThOE pm 02:50 **Rapid chemical characterization of microplastics and nanoplastics by thermal desorption and pyrolysis mass spectrometry with semi-supervised learning;** Thomas P. Forbes¹; John Pettibone¹; Eric Windsor¹; Diana L. Ortiz-Montalvo¹; Abigail P. Lindstrom¹; Joseph M. Conny¹; Robert A. Fletcher¹; ¹National Institute of Standards and Technology, Gaithersburg, MD

ThOE pm 03:10 **Combining high-performance liquid chromatography with chemical ionization tandem mass spectrometry by liquid electron-ionization interface to determine per- and polyfluoroalkyl substances;** Malvika Dutt¹; Adriana Arigo¹; Giorgio Famigliini¹; Pierangela Palma^{1,2}; Achille Cappiello^{1,2}; ¹UNIVERSITY OF URBINO CARLO BO, URBINO, Italy; ²Vancouver Island University, Nanaimo, BC

ThOE pm 03:30 **Odor profiling and SIFT-MS analysis reveal relationships for perceived odor during wastewater treatment;** Michael A McGinley¹; Olivia Rice¹; Leslie P. Silva²; ¹St. Croix Sensory, Inc., Stillwater, MN; ²Syft Technologies, Los Angeles, CA

ThOE pm 03:50 **Resolving halogenated water disinfection by-products (DBPs) isomers of Bisphenol A with ion mobility - mass spectrometry;** Mauricio Marques Dos Santos¹; Caixia Li¹; Shenglan Jia¹; Shane A Snyder¹; ¹Nanyang Technological University (NTU)- NEWRI, Singapore, Singapore

ThOE pm 04:10 **Improved target, suspect- and non-target analysis of environmental contaminants using a GC-EI&CI-TOF-MS system;** Marleen Vetter¹; Steffen Bräkling¹; Sonja Klee¹; ¹TOFWERK, Gwatt (Thun), Switzerland

ThOF pm: Lipidomics: Targeted and Untargeted General Assembly A

Session Chair: Kermit Murray (Louisiana State University)

ThOF pm 02:30 **Development of a targeted multiplexed method to measure sphingolipids in CSF samples from patients with multiple sclerosis;** Yadira X Perez Paramo¹; Dawn Dufield²; Rathna Veeramachaneni²; Emily Parkhurst²; Christopher Harp¹; Akshaya Ramesh¹; W. Rodney Mathews¹; Veronica Anania¹; ¹Genentech, South San Francisco, CA; ²KCAS, Olathe, KS

ThOF pm 02:50 **Quantitation and Structural Elucidation of Intact Brain Sphingolipids with nanoflow HPLC-MS/MS;** Ryan L Schindler¹; Jennyfer Tena¹; Carlito B. Lebrilla¹; ¹UC Davis, Davis, CA

ThOF pm 03:10 **Ultraviolet photodissociation (UVPD) mass spectrometry for structural characterization of lipids in biological matrices on chromatographic time scales;** Rahul Ravi Deshpande¹; Mandy Bowman¹; Bashar Amer¹; Thomas Moehring²; Susan Bird¹; ¹Thermo Fisher Scientific, San Jose, California; ²Thermo Fisher Scientific, Bremen, Germany

ThOF pm 03:30 **Connecting altered branched fatty acid distributions with membrane fluidity in daptomycin-resistant Staphylococcus aureus;** Christian D Freeman¹; Craig Gatto²; Brian J Wilkinson²; Vineet K Singh³; Kelly M Hines¹; ¹University of Georgia, Athens, GA; ²Illinois state

THURSDAY ORALS

- ThOF pm 03:50 *university, Normal, IL; ³A.T. Still Univeristy, Kirksville, MO*
Structural Characterization of Phosphatidylcholine Isomers Using Collisional Induced Dissociation/Electron Induced Dissociation (CID/EID) in Imaging Mass Spectrometry; [Tingting Yan](#)¹; Zhongling Liang¹; Boone M. Prentice¹; ¹University of Florida, Gainesville, FL
- ThOF pm 04:10 **Investigating the lipidome of small extracellular vesicles;** [Adriana Zardini Buzatto](#)¹; Liang Li^{1, 2}; ¹The Metabolomics Innovation Centre (TMIC), Edmonton, AB; ²University of Alberta, Edmonton, AB

ThOG pm: Forensics: Innovations and Applications General Assembly B

Session Chair: [Alyssa Marsico](#) (University of New Haven)

- ThOG pm 02:30 **Forensic proteomics offers a new minimally invasive and robust tool for discriminating ivory species;** [Catherine Gilbert](#)¹; Vaclav Krupicka¹; Aleksandra Popowich²; Katell Bathany¹; Stéphane Claverol³; Julie Arslanoglu²; Caroline Tokarski¹; ¹Institute of Chemistry and Biology of Membrane and NanoObjects (CBMN), CNRS UMR 5248 University of Bordeaux, Bordeaux, France; ²Department of Scientific Research, The Metropolitan Museum of Art, New York City, NY; ³Proteome Platform, University of Bordeaux, Bordeaux, France
- ThOG pm 02:50 **Trace Detection of Styphnate and Fulminate Primary Explosives via LC-MS/MS;** [Sarah N Sipe](#)¹; Haley A Mulder¹; Courtney A Cruse¹; Mark L Miller²; ¹ORISE Visiting Scientist Program - FBI, Quantico, VA; ²Federal Bureau of Investigation, Quantico, VA
- ThOG pm 03:10 **High Throughput Analysis of Isomeric Drug of Abuse in Human Urine Samples by Liquid Chromatography Vacuum Differential Mobility Spectrometry-Mass Spectrometry;** Maria Fernanda Cifuentes Girard¹; Patrick Knight²; [Gerard Hopfgartner](#)¹; ¹University of Geneva, Geneva 4, Switzerland; ²Shimadzu Research Laboratory (Europe), Manchester, United Kingdom
- ThOG pm 03:30 **A Modified 3D-Printed Cone Spray Ionization (3D-PCSI) Source for On-Site, Trace Forensic Evidence Processing via Integrated Vacuum Collection;** [Christopher C. Mulligan](#)¹; Ebenezer E. Bondzie²; Adewale A. Adehinmoye²; Brian T. Molnar³; Patrick W. Fedick³; ¹Illinois State University, Normal, IL; ²Illinois state university, Normal, IL; ³Naval Air Warfare Center, Weapons Division, China Lake, CA
- ThOG pm 03:50 **Characterizing the likelihood of misidentifying fentanyl analogs using the NIST23 EI-MS Library;** [Arun Moorthy](#)¹; Edward Erisman¹; Anthony Kearsley¹; Yuxue Liang¹; Edward Sisco¹; William E. Wallace¹; ¹NIST, Gaithersburg, MD
- ThOG pm 04:10 **Drug of abuse Screening in nail at 8 Seconds per samples Using LDTD-MS/MS;** [Sarah Demers](#)¹; Jonathan Rochon²; Serge Auger²; Jean Lacoursière²; Pierre Picard²; ¹Phytronix Technologies, Quebec City, QC; ²Phytronix Technologies Inc., Quebec, CA
- ThOH pm 02:50 **Scalable analysis of untargeted LC-HRMS data by means of SQL database archiving;** [Marie Mardal](#)^{1, 2}; Brian Schou Rasmussen²; Kristian Linnet²; Christian Brinch Mollerup²; ¹Department of Pharmacy, the Arctic University of Northern Norway, Tromsø, Norway; ²Department of Forensic Medicine, University of Copenhagen, Copenhagen, Denmark
- ThOH pm 03:10 **Bayesian statistical modeling reveals missing value mechanisms in label-free Mass Spectrometry-based proteomics experiments;** [Devon Kohler](#)¹; Olga Vitek¹; ¹Northeastern University, Boston, MA
- ThOH pm 03:30 **Molecular networking for the 21st century;** [Christoph A. Kretzler](#)¹; John T. Prince¹; Daniel G. C. Treen¹; David Healey¹; Joe Rokicki¹; ¹Enveda Biosciences, Boulder, CO
- ThOH pm 03:50 **A Novel Method for Automatically Calibrating GC Retention Index from MS Library Search Results;** [Don Kuehl](#)¹; Stacey Simonoff¹; Yongdong Wang¹; ¹Cerno Bioscience, Las Vegas, NV
- ThOH pm 04:10 **Boosting workflow efficiency and productivity with instrument intelligence and smart automation;** [Emma E. Rennie](#)¹; Huy Bui¹; Patrick Batoon¹; Christian Klein¹; James S. Pyke¹; Li Sun¹; Haopeng Wang¹; George Yefchak¹; ¹Agilent Technologies, Inc., Santa Clara, CA

ThOH pm: Informatics: Innovations General Assembly C

Session Chair: [Xiuxia Du](#) (University of North Carolina at Charlotte)

- ThOH pm 02:30 **LibGen 2.0: fully automated pipeline for cleaning spectral libraries;** [Fanzhou Kong](#)¹; Uri Keshet¹; Jeremiah D Wells¹; Oliver Fiehn¹; ¹West Coast Metabolomics Center, University of California, DAVIS, CA

MONDAY WORKSHOPS, 5:45 – 7:00 PM

Mon Workshop 01 The Role of Mass Spectrometry in Emerging Energy Technologies Development *Energy Petroleum & Biofuels Interest Group*

Presiding: Yuri Corilo, Leonard Nyadong

Room 310A

Alternative and emerging energy technologies including batteries, hydrogen, nuclear and renewables such as solar, wind, hydropower, geothermal and biofuels all play a crucial role in the future of our planet. They provide a sustainable solution to our growing energy demands while reducing our dependence on finite resources such as oil and gas. From an economic perspective, alternative energy technologies can lead to reduced energy costs, increased energy security, and new job opportunities in the energy industry. Finally, from an industrial perspective, the development and use of emerging energies can lead to technological advancements and innovations in the energy sector, contributing to the growth of the global economy.

Mass spectrometry technology has played a key role over several decades in the development of fossil fuels and to a lesser extent, alternative energies including biofuels. Mass spectrometry allows for the precise analysis of chemical compounds, which provides the detailed molecular composition of energy feedstock materials. The information is essential for optimizing the energy source production and refining processes, leading to more efficient and cost-effective energy generation. Mass spectrometry is beginning to play a role in developing new energy technologies, such as advanced batteries and fuel cells, by enabling scientists to analyze and improve their performance properties.

This workshop will provide the opportunity to discuss the role of mass spectrometry in development of alternative energy technologies. The workshop will feature practitioners who are applying mass spectrometry in alternative energy research to discuss experiences, enablers, challenges, and the outlook of the role of mass spectrometry in emerging energy fields.

Mon Workshop 02 Nucleic Acids Mass Spectrometry: Emerging Applications, Effective Analytical Strategies, and Characterization for Progressively Larger Nucleic Acids *Oligonucleotides and Nucleic Acids Interest Group*

Presiding: Varun Gadkari, Jennifer Lippens, Robert Ross

Room 310BC

Recently, nucleic acids have returned to the forefront of biomedical research, with rapidly growing interest in fundamental, translational, and pharmaceutical research areas. Scientists are seeking new and improved methods for characterizing challenging and relevant, nucleic acid targets and therapeutics, including oligonucleotides ranging in size from antisense oligonucleotides to mRNA. This interest group seeks to bring together ASMS members across multiple sectors to discuss the latest in nucleic acid mass spectrometry including sample production and preparation, method development, analysis strategies, application needs, and more. Long-term, the goal is to foster a strong community in this space and accelerate the development of mass spectrometry-based strategies for nucleic acids research.

Our 2023 format will consist of 4-5 panelists from diverse backgrounds and including both mid-to-late stage career established researchers as well as junior/early career scientists to provide exposure for emerging researchers. Panelists will present a short intro of their current research followed by a moderated open discussion/question and answer session over the presentations and any other questions that attendees may bring forward. We will also gauge interest for a future Asilomar Meeting focusing on nucleic acids through participant surveying and gather feedback on topics surrounding nucleic acid mass spectrometry that would be of interest for future ASMS workshops. We look forward to workshop participants coming with their most burning questions and to a great discussion in this exciting space.

Mon Workshop 03 Research and Funding Opportunities at the FDA: Mass Spectrometry for Drug Product Quality *Independent*

Presiding: Jinhui Zhang Zhang, Mack Shih

Room 320A

The purpose of this workshop is to provide mass spectrometry researchers in academia a broader picture of the importance of mass spectrometry in drug evaluation and research, as well as protecting public health at the FDA. The workshop will start with a set of quiz/poll to check the attendees' knowledge on small and large molecule drugs discovery, development, evaluation, and the role of mass spectrometry in each of the stages. Then, we will share with the attendees several research "stories" we accomplished in the past several years as case studies to highlight how we implement advance mass spectrometry and automation tools at the FDA to: 1) address carcinogenic drug impurities to protect public health; 2) support the modernization of over-the-counter drug products; 3) enable quality surveillance of marketed drug products; 4) help to clarify the current guidance; and 5) advance drug evaluation practice through research. In the end, we will discuss how academic researchers can contribute to FDA's drug product quality research through different funding mechanisms.

MONDAY WORKSHOPS, 5:45 – 7:00 PM

Mon Workshop 04

Global participatory efforts to characterize the biochemical composition of food: The Periodic Table of Food Initiative and The Proteomes that Feed the World

Independent

Presiding: Jessica Prenni, Bernhard Kuster

Room 320BC

Food is at the center of addressing some of the world's most urgent challenges. However, our scientific understanding of the biochemical composition of food and the organisms that underlie it is rudimentary at best. This workshop will present two global efforts focused on improving our understanding of what is in our food. (1) The Periodic Table of Food Initiative (PTFI) is developing standardized, fully democratized LC-MS based technology platforms for generating comprehensive food composition data. These platforms are open-source and can be used by laboratories around the world to populate a reference database that enables open access and comparability of foodomics data. (2) The Proteomes that Feed the World (PFW) is mapping the proteomes of all major tissues and organs of the 100 crop plants most important for human nutrition. This effort will create a Crop Proteome Atlas of high value to academia as well as the agricultural and food industries. The objectives of this workshop will be to: (1) introduce the PTFI and the PFW to the broader mass spectrometry community; (2) provide updates on progress as well as spark innovative ideas and feedback and (3) discover new opportunities for engagement.

Mon Workshop 05

Single-Cell Proteomic Standardization: From Study Design to Data Analysis

Independent

Presiding: Jennifer Van Eyk, Peter Nemes

Ballroom A

Recent advances in mass spectrometry technology have extended proteomics into single cells. A rapidly growing number of laboratories seek to adapt single-cell mass spectrometry across a broad swath of biology. Technologies based on automated sample preparation, liquid chromatography and capillary electrophoresis as well as mass spectrometry have enabled ultra-high sensitive quantification of hundreds-to-thousands of proteins in various cell types. These studies are revealing previously unknown (and unexpected) paradigms about the molecular organization of the cell. Yet there are many challenges associated with the design, execution and data analysis of single-cell proteomics. To facilitate scientific rigor and reproducibility, we propose a single-cell proteomics workshop. This workshop will fulfill the following aims: (1) Update the scientific community of technological advances with a focus on study design, execution, and data analysis; (2) disseminate single-cell methods and protocols to promote technological adaptation with a focus on recent community-wide standards established in single-cell mass spectrometry proteomics; (3) identify remaining challenges in single-cell proteomics; (4) recruit new members to the field. The workshop will focus on challenges and solutions. It will start with each panelist giving a 5 min talk overview of their biggest challenge and solutions and end with a roundtable discussion of panelists, who will solicit and answer questions from attendees. Moderator, Jennifer Van Eyk. Panelists: Nikolai Slavov (Northeastern U.) - Study design and Standards; Lingjun Li (U. of Wisconsin) - Sample prep; Ryan Kelly (Brigham Young Univ) - sample integration with MS; Peter Nemes (U. of Maryland) - MS throughput; Fabio Gomes (Scripps) - Topdown SCP; Olga Vitek (Northeastern Univ) - Statistics with respect to SCP.

Mon Workshop 06

Networking for Scientists: Celebrating Women Mass Spectrometrists

Independent

Presiding: Stacy Malaker, Aivett Bilbao, Julie Courraud

Ballroom B

This year we plan on having a more interactive networking event. To begin, as in years past, 3-4 new panelists will be introduced and then take time to discuss career paths they have followed, what factors they considered when making big decisions, and advice they would give to a woman and members from underrepresented minorities facing the same challenges. Then, we will ask the attendees to answer questions via Kahoot (or similar polling application), which the panelists will then comment on and discuss. The goal here would be for the participants to see they are not alone in their experiences and/or challenges. Some example questions for this event could include:

- Has there been a time you felt seen and supported as a woman in your field?
- Do you feel like you have a positive network/support system at work or your program?
- Do you have a mentor you can look up to or help you navigate career challenges?
- Have you looked for networking experiences with other women in STEM?
- Have you seen improvements to promote gender equality and diversity inclusion within your team/group?

Following this, a larger cohort of organizers/volunteers (approximately 15-20) of varying backgrounds and career stages will then lead small group discussions. The attendees will be encouraged to join a group, share their experiences and contact information, then network accordingly. The small group discussions will last for the remainder of the workshop before the gap hour networking sponsored by Agilent.

MONDAY WORKSHOPS, 5:45 – 7:00 PM

Mon Workshop 07 Exploring the World of Mass Spectral Libraries, Library Search Software and Their Applications *Mass Spectral Libraries Interest Group*

Presiding: Emma Rennie, Xiaoyu Yang, Melinda McFarland

Ballroom C

The growing amount of data produced by mass spectrometry has made the identification of compounds in routine data analysis increasingly challenging. The use of mass spectral (MS) libraries has emerged as a valuable solution for fast and accurate compound identification. This workshop delves into the most recent advancements in MS libraries, exploring their use, application, and accompanying software tools. A panel of leading experts will present on the current state of MS libraries and the software tools they have developed or utilized in their work. They will also provide their perspectives and insights on the development and application of MS libraries. Following their presentations, there will be an opportunity for a brief Q&A session, followed by an interactive discussion on a range of topics, such as: the available MS libraries; library search software; integration with open source software platforms (e.g. Skyline and GNPS); AI applications; data processing software for searching and library building; and the use of libraries in areas such as metabolomics, food science, clinical proteomics, and environmental analysis. By the end of the workshop, participants will have a comprehensive understanding of how MS libraries can enhance their data analysis and the wide variety of software tools that can support this process.

Panelists: Michael MacCoss (University of Washington), Stephen Stein (NIST), Lloyd Sumner (University of Missouri), Arpana Vaniya (UC Davis), Mingxun Wang (UC Riverside).

Mon Workshop 08 Ion traps as reaction vessels *Ion Trap MS Interest Group*

Presiding: Dalton Snyder, Lucas Szalwinski

Room 332

Ion traps are remarkably versatile analytical devices. They are capable of a wide range of capabilities that other analyzers can only dream of, from ion isolation to mass analysis and a full suite of MS/MS experiments. But that's not all! Ion traps can also serve as clean, selective, fast, and efficient reaction vessels for squeezing every ounce of chemical and structural information out of analytes.

This year's Ion Trap MS workshop will focus on the ion trap's ability to serve as a vessel for conducting ion/ion, ion/molecule, ion/photon, and fragmentation reactions. A diverse selection of speakers from academia and industry will give lightning talks on reactions of all sorts. These talks will then be followed by a panel discussion with audience Q & A.

Mon Workshop 09 Career Opportunities for Chinese Students and Scholars *Independent*

Presiding: Junmin Peng, Shuguang Ma

General Assembly A

With the rapid development of mass spectrometry technologies and the increasing applications to academic research, medicine, industry, and regulatory agencies, a growing number of mass spectrometrists including thousands of Chinese students and scholars are trained. The workshop for Career Development Opportunities for Chinese Students and Scholars aims to provide career perspectives to students and scholars to learn the career paths at different career stages. We will invite four speakers from academia, clinic, industry, and regulatory agencies to share their experiences for career development. We will also assemble a group of discussion panelists to answer questions from the audience. We believe the workshop is beneficial to both students and scholars of all ASMS members and potential employers. The workshop will provide opportunities for students and scholars to prepare for their career development during and after mass spectrometry training and help them to set up career goals in the field of mass spectrometry.

Mon Workshop 10 Making Top-Down Mass Spectrometry Easier to Develop and Apply: Ways to Work Together and How Everyone Can Contribute

Top-Down Proteomics Interest Group

Presiding: Yuri van der Burgt, Mowei Zhou

General Assembly B

Top-down mass spectrometry (TDMS) provides unique and complementary information at the intact protein level that is commonly masked when using bottom-up proteomic methods. Nevertheless, the community has experienced various challenges in adopting TDMS strategies due to a lack of a "one size fits all" solution. The difficulty is exacerbated by many options for sample preparation protocols, instrument parameters, and data analysis software, especially when dealing with complex samples. After the feedback from the 2022 workshop, the Consortium for Top-down Proteomics (CTDP) has established an Early Career Researcher (ECR) committee to help identify opportunities and plan activities to address many of these challenges as a community.

In this workshop, we will first have ECR representatives: 1) present planned near-term activities about more expertise sharing, including experimental protocols; 2) discuss the vision for the newly opened CTDP LinkedIn group for barrier-free communication; 3) discuss an initiative to create "golden datasets" for software development with inputs from the community; 4) solicit ideas for further improvements and new activities. This will be followed by an update about the CTDP initiative on an interlab study of capillary electrophoresis from Alexander Ivanov, Liangliang Sun, and Kevin Jooss. Last, we will host an open panel discussion for the audience to ask questions and suggest ideas.

MONDAY WORKSHOPS, 5:45 – 7:00 PM

Lastly, we will invite two newcomers to the field to discuss future TDMS applications with the audience, with the goal of inspiring new ideas and collaborations.

Mon Workshop 11 **New Aspects in the Development and Implementation of Multi-Attribute Method (MAM)**

Biotherapeutics Interest Group
Presiding: Da Ren, Andrew Mahan
General Assembly C

The advances of new indication and therapeutic modalities in the pharmaceutical industry drives the development of new analytical methods that provide enhanced content in a more efficient manner. In the past of decade, liquid chromatography (LC)-mass spectrometry (MS)-based Multi-Attribute Method (MAM) has successfully demonstrated its capability in replacing traditional chromatographic, electrophoretic, and binding assays for monitoring both product and process quality attributes (Rogers R. et al., AAPS J, 2017, Ren D., Trends Biotechnol. 2020).

As we enter a new decade of technology and method development, MAM's utility is expanding. Recent advances in mass spectrometry instrumentation have provided novel opportunities in reforming the original MAM. The industry-wide MAM Consortium inspires method development and diversity for new MAM approaches that are fitting into different application in biopharma R&D schemes. New approaches to MAM are emerging, e.g. fully automatic sample preparation, MAM for cell and gene therapies, compact MS for MAM in QC, and new data acquiring approaches. The biotherapeutic interest group workshop offers a forum for members to share and discuss those new aspects in the development and implementation of MAM.

Mon Workshop 12

Data quality in the core lab: Preventing, catching, reporting and sometimes even fixing! suboptimal "bad data" in a omics core facility aka the "Bad data Workshop"

Analytical Lab Managers Interest Group
Presiding: Brett Phinney, Uri Keshet, Dave Quilici
Room 340AB

Bad samples, bad data? Data quality in the omics core lab is a challenging task because of the large-scale and untargeted nature of omics experiments, and the variety of instruments and assays that a core lab is expected to provide. Some of the causes for bad data are Sub optimal sample prep , miss behaving LC's, and Mass spectrometers on the verge of blowing up. While there are ways to minimize bad data, it still happens, and it happens more than we like. Come to the workshop and share tips and strategies for preventing and, if necessary, dealing with bad data in both proteomics and metabolomics core facilities. After a few brief examples from our speakers, audience members will be given a shoulder to cry on or asked to share their strategies for dealing with BAD DATA

Mon Workshop 13

Emerging Techniques for Rapid Fabrication in MS Laboratories

Independent
Presiding: John F. Cahill, Vilmos Kertesz
Room 351ABDE

The use of additive and subtractive manufacturing, as well as open-source electronic prototyping platforms, has become increasingly prevalent in scientific research, including in the field of MS. These technologies allow for rapid prototyping of components and devices, which can greatly enhance the efficiency of the research process. In the workshop series, participants will share their experiences with designing and fabricating custom components. We will also discuss the use of open-source electronic prototyping platforms such as Arduino or Raspberry Pi to develop custom electronics for instrument control and data acquisition. Participants can share best practices and their best 'tips and tricks' for designing and prototyping components quickly and efficiently. Overall, the workshop series will be a valuable opportunity for MS researchers to share knowledge and expertise related to the use of these auxiliary technologies, with the goal of advancing research in the MS field.

MONDAY WORKSHOPS, 5:45 – 7:00 PM

Mon Workshop 14 Cannabis & Hemp Science: The Importance of Mass Spectrometry *Independent*

Presiding: Jordan Witkop
Room 351CF

The global legalization of cannabis and hemp-derived medicine and consumer products has paved the way for advances in cannabis science from the accurate detection of active cannabinoids and harmful, trace contaminants to more informative strain typing, advanced breeding programs and clinical research. GOALS: Deliver key opinion leader panel discussions on novel applications of cannabis and hemp in the medical arena as well as future directions. Foster discussions regarding the applications of mass spectrometry to cannabis and hemp science and research. Encourage expanded use of mass spectrometry in cannabis/hemp applications by sharing information and discussing emerging growth areas.

Panelists:

- Brett Ginsburg, PhD (START Center Genetic Research Professorship Department of Psychiatry, The University of Texas Health Science Center at San Antonio) "Using Mass Spec to evaluate recreational and medical cannabinoid use in clinical samples."
- Russell W. Jessup, PhD (Associate Professor of Perennial Grass & Industrial Hemp Breeding Department of Soil and Crop Sciences, Texas A&M University) "Developing high-throughput & low-cost chemotyping tools"
- Matt Vergne, PhD (Associate Professor, Dept of Pharmaceutical Science, Lipscomb University) "Development of a cannabinoid testing method using blood plasma collection cards and LC-MS/MS"

Mon Workshop 15 Mind the (Translation) Gap *Clinical Chemistry Interest Group*

Presiding: Brian Rappold
Room 360ABDE

The ASMS annual meeting is replete with novel technologies, new biomarkers and evolving means to assess diseases in patients. However, the path to utilize these innovations in the clinical environment is not a common point of discussion. This workshop will discuss the framework of translating an innovation into reality with a panel of experts in diagnostic medicine, including representatives from manufacturers of FDA-approved materials and assays, venture capital/biotech investment and international reference labs. A discussion of the regulatory and financial environment will take place with a "Shark Tank"-like approach; imaginary proposals will be offered to the panel to launch a conversation about bridging the gap from a discovery to a deployment in a diagnostic laboratory.

Mon Workshop 16 Exposome research: overcoming challenges to deliver answers *Exposomics Interest Group*

Presiding: Benedikt Warth, Ruth Marfil-Vega, Silvia Balbo
Room 360CF

The workshop will inform and discuss the latest developments in the expanding field of exposome research. An overview of the latest technological developments and global initiatives will be presented.

The discussion will focus on the tools, infrastructure, and support necessary to continue successful exposomics research. This includes comprehensive mass spectrometric and bioinformatic workflows. Researchers from renowned labs working in the area will be present to share their views on current shortcomings (infrastructure, standardization, harmonization, chemical coverage, sensitivity issues) but also share their vision of how true omic-scale exposure assessment can be successfully established. Future directions of exposomics will be discussed in light of a massive push coming from both, US-based and European initiatives leading the way toward innovative research in the arena of environmental health and public and personalized prevention.

Mon Workshop 17 Using Casanovo for de novo peptide sequencing *Independent*

Presiding: Melih Yilmaz, William Noble, Will Fondrie
Room 361ABDE

Casanovo is a new de novo peptide sequencing method that uses a deep learning model trained on massive data to achieve very high prediction accuracy. The software is implemented in Python and is available open source with an easy installation procedure. The goal of this hands-on workshop is to train users to install the software, run Casanovo using a pre-trained trypsin or non-enzymatic model, and interpret and visualize the results. We will also show you how to fine-tune the model with data from your own lab to make Casanovo work well for you. Attendees may wish to bring their own laptops to follow along with the demos. The workshop will close with a discussion of the pros and cons of de novo sequencing, with the aim of eliciting feedback for improving the utility of Casanovo and other similar tools for the user community.

TUESDAY WORKSHOPS, 5:45 – 7:00 PM

Tues Workshop 01 **Open and Reproducible Data Analysis for FT-MS** ***FTMS Interest Group***

Presiding: David Butcher, Yuri Corilo
Room 310A

The proposed FT-MS interest group workshop will focus on applying open and reproducible workflows to analyze FT-MS data. It will build on the designation of 2023 as the Year of Open Science by the White House Office of Science and Technology Policy. While the general subjects of open science and FAIR data will be mentioned, the workshop's primary focus will be practical methods that researchers can use to ensure that the analysis of data collected using FT-MS instruments can be effectively shared and reproduced by other researchers. This will include using computational workflows implemented in open-source programming languages such as Python and R, workflow languages, containerization technologies, metadata capture and standards, and other existing and emerging methods. The exact content of the workshop will be at the discretion of the speakers, who will have expertise in software and workflow development for FT-MS data analysis.

The workshop will consist of a 15-minute introduction given by the co-chairs, followed by three 10-minute talks/demonstrations given by the recruited speakers on a specific aspect or example of reproducible analysis of FT-MS data. In the final 30 minutes, questions will be taken from the audience.

The overall goals are to:

1. Provide researchers with experience in computer programming and practical advice in making their data analyses open and reproducible.
2. Communicate to researchers without computer programming skills the value gained from implementing reproducible data analysis practices.
3. Promote the use of these practices in the FT-MS community.

Tues Workshop 02 **Accelerator Mass Spectrometry (AMS): Current Utility and Future Opportunities** ***DMPK Interest Group***

Presiding: Lina Luo, Holly Maw
Room 310BC

The human radiolabeled adsorption-distribution-metabolism- excretion (ADME) study provides a quantitative and comprehensive overall picture of the disposition of a drug and is required for new drug approval. The accelerator mass spectrometry (AMS), which enables microtracer and microdosing studies, to ultrasensitively quantify radiolabeled compounds in biological matrices, offers various strategic advantages in drug development. Advanced AMS technology allows administration of 100-fold to 1000-fold lower amounts of carbon-14, which significantly reduces radiation burden to human volunteers. With microtracer hADME studies, the safety of trial participants is greatly improved as well as the need for a GMP grade drug substance can be eliminated. This is especially critical in vulnerable populations, such as pediatric or pregnant subjects, which further reinforce the need to keep radiation burden to a minimal level. AMS further facilitates innovative approaches for study designs to allow dosing by alternative dose routes. Administration of drug via routes such as ocular and dermal can be introduced with the sensitivity of AMS. With the AMS-enabled ADME study, we can have data on a complete metabolic profile in circulation and excreta earlier than the currently well-established timeline (before end of Phase II). Overall, the drug development timeline can be accelerated with the AMS-enabled ADME study, and a complete understanding of drug disposition can be achieved earlier. This workshop will bring together established researchers from the pharma industry and research institution to discuss current utility and future opportunities of the AMS technology in drug development.

Tues Workshop 03 **Constructing an Individual Development Plan (IDP)** ***Career Development Interest Group***

Presiding: Troy Wood
Room 320A

The concept of the Individual Development Plan (IDP) is employed frequently in industrial settings to help employees construct a definitive plan for achieving career goals; however, IDP can be used in any work setting. In 2003, the Federation of American Societies for Experimental Biology (FASEB) proposed an IDP framework for postdoctoral fellows; subsequent polling of postdocs who developed an IDP reported it helpful to self-assess their abilities and skills, and identify which skills they would need for career advancement. Borrowing this framework, we will provide an overview of developing an IDP: 1) self-evaluation of skills, interests, and values, 2) use the self-assessment as a guide to evaluate and explore career opportunities (including alternative options), 3) setting specific goals for the aspired-to career path, including discussion with mentors, and 4) putting the IDP into place. We hope the workshop will either lead to the formulation of individual IDP or will refresh thoughts to those with existing IDPs. Although geared toward young mass spectrometrists, members from any stage of their career are welcome.

TUESDAY WORKSHOPS, 5:45 – 7:00 PM

Tues Workshop 04 **The NIH and NSF Review and Funding Process** *Independent*

Presiding: Salvatore Sechi, Kelsey Cook, Douglas Sheeley, Kenneth Ryan
Room 320BC

Many ASMS members and conference participants are supported by the National Institutes of Health and the National Science Foundation. During this workshop the general funding and review process of grant applications/proposals will be presented. Issues like identifying the best contacts, writing an effective application/proposal, and responding to the reviewers' criticisms will be discussed. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on new investigators and training opportunities. Tips on grant writing and insights into the review process will be presented. The session will also provide an opportunity to inquire about the latest NIH and NSF initiatives and priorities. Substantial time will be allotted for discussion and questions. NIH and NSF staff will also be available for individual discussions with investigators during scheduled "Office Hours" in the poster exhibit hall.

Tues Workshop 05 **From data to biology: using -omics datasets to generate an unbiased hypothesis** *Bioinformatics MS Interest Group*

Presiding: Katarzyna Kulej, Claire O'Donovan
Ballroom A

This workshop will discuss the common practices to "break the ice" in data simplification and interpretation. Most ASMS conference attendees deal with large datasets that require processing, sorting, filtering, and representation. Is there a rulebook for approaching these tables? The answer is no. However, we will discuss some of the most used and accepted workflows for interpreting an -omics dataset and how best to approach data representation. We will focus on both understanding the quality of MS-data output and reducing the complexity of biological data extracted. At the end of this session, we expect attendees to have acquired tips and tricks to minimize the activation barrier facing -omics data interpretation.

We will present some of the most commonly used and freely available software to interpret proteomic data and display data graphically. We will focus on how to analyze proteomes, including their protein post-translational modification (PTM), without needing a driving hypothesis. Furthermore, we will introduce the repositories used to match newly generated data with pre-existing knowledge on gene/protein/PTM biodata and how to cross-validate novel findings with what is reported in the literature. Finally, we will open a roundtable discussion of the most common issues and bottlenecks in data interpretation. We will welcome different perspectives, ideas, and practices in unbiased hypothesis generation using -omics datasets. Ultimately, our overall goal is to encourage non-experts in bioinformatics to explore user-friendly resources for MS data analysis.

Tues Workshop 06 **Recognizing the "A" in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists** *Membership, Diversity, and Inclusion Committee*

Presiding: ASMS Membership, Diversity, and Inclusion Committee Members
Ballroom B

Accommodations for persons with disabilities are rarely implemented with a "one-size fits all approach" as disabilities can be multi-faceted, range in severity, vary in impact based on the setting, and be classified as visible or non-visible in nature. Accessibility barriers, especially those experienced in a laboratory or workplace environment, can stifle knowledge exchanges, limit collaboration and participation, or reduce a scientist's quality of life. It is therefore important to promote a work culture where every member is appreciated, respected, and given the tools to succeed. Dialogue is the first step in recognizing the needs of persons with disabilities and formulating effective accommodation ideas.

The ASMS Membership, Diversity, and Inclusion (MDI) committee will host the first ASMS workshop on accessibility. To address the needs of visible and non-visible disabilities, the workshop program will be divided into 3 segments that highlight physical, sensory, and cognitive disabilities. The workshop format will feature a panel composed of students, post-docs, faculty, and staff that will speak to the unique issues experienced by persons with disabilities as well as evidence-based solutions that have been implemented to make laboratories and work environments more accessible.

Tues Workshop 07 **Data Independent Acquisition: After the Acquisition** *Data Independent Acquisition Interest Group*

Presiding: Lindsay Pino, Lukas Reiter
Ballroom C

Data independent acquisition (DIA) has drawn the interest of (prote)omics researchers thanks to its high levels of reproducibility, capacity for large sample sizes, and the completeness of quantitative data. As academia and industry strives towards scaling workflows to hundreds or thousands of samples, derived from single cells, cell line screens, or large clinical cohorts, the boundaries of throughput and proteome depth are rapidly increasing, requiring advances in liquid chromatography-mass spectrometry systems and bioinformatics to support the scope of experimentation.

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In this workshop, we invite experts in the field to discuss topics of importance and debate amongst DIA users. We explore both fads and trends that are emerging as DIA opens proteomics to larger and larger data, with a focus on what happens after acquisition, from preliminary data processing to data storage to formatting and data interpretation and dissemination. This includes the use of deep learning to better process DIA on the level of spectra but also on the level of interpreting large scale sample cohorts. Further, we are going to discuss how the next 10 years of DIA may look like or what users would like to see developed in the next 10 years. Along these lines, we'll revisit some of the topics from previous DIA workshops to compare the direction the field seemed to be going to where things ended up going. For example, the prediction last year was that "more peptide/protein detections" would be this year's great breakthrough, stemming from increased use of AI/ML in data analysis. We will also explore new applications for DIA, or the lack of new applications, to evaluate where DIA is being most heavily used versus applications that are still challenging for DIA approaches.

Tues Workshop 08 **FAIR Data Sharing Principles and Barriers: the New NIH Data Management and Sharing (DMS) Policy** **Metabolomics Interest Group**

Presiding: Tytus Mak, Thomas Horvath, Maryam Goudarzi
Room 332

As of January 2023, all National Institutes of Health (NIH) funded investigators are required to abide by the new NIH Data Management and Sharing Policy (DMS). This policy requires new proposals to include a data management plan, and experimental data generated using NIH funds to be Findable, Accessible, Interoperable, and Reproducible, or FAIR. FAIR data sharing is integral to spur research reproducibility, promote data reuse, and accelerate research. The meeting will open with a few opening remarks regarding the theme of the meeting, a short introduction for each of the speakers, and a short Slido poll regarding the challenges facing the community and suggestions for the ASMS 2024 meeting topic (5-10 mins). The first speaker will be Dr. Reed Shabman, Program Officer at NIH-NIAID (or another NIH representative), who will comment on the implementation of the new DMS policy (15 mins). Then, a short presentation (15 mins) on the advantages, obstacles, and solutions of FAIR Data Sharing in scientific research will be presented by Dr. Laura Hughes (Scripps Research). Then, attendees will be asked to form small groups to discuss the obstacles and potential solutions for complying with the DMS policy in their respective laboratory environments (20 mins). The balance of the time will be spent discussing the findings discussed in each of the small group interactions (~15-20 mins).

Tues Workshop 09 **Kahoot Trivia! LCMS (and other topics)** **LCMS & Related Topics Interest Group**

Presiding: James Dodds, Jack Ryan, Karen Butler
General Assembly A

For the past couple of years we've been hosting a phone based trivia evening where attendees can login to a free app (Kahoot) and play along with trivia questions against their friends for enjoyment and the top 3 players get prizes (usually stuffed animals like microbes and such).

Our attendance last year was something like 80 people, not sure how that stacks up to the other workshops. Maybe it was Monday/Tuesday night, can't recall.

Tues Workshop 10 **Lipidomics: What does International Lipidomics Society offer to the lipidomic community?** **Lipids & Lipodomics Interest Group**

Presiding: Michal Holcapek, Jeffrey McDonald
General Assembly B

The lipidomics community is growing, and many newcomers are joining or at least using the lipidomics data in their research. However, there are not yet standardized methods for lipidomic analyses and data reporting, which may sometimes lead to confusion. The International Lipidomics Society (ILS) was established in 2019 with the goal of fostering the cooperation of lipidomic researchers and harmonizing methodologies, nomenclature, data reporting, and organization of ring trials. This lipidomics workshop has two main objectives. First, we would like to introduce the key activities of the ILS, such as the harmonization of lipidomics workflows with the help of minimum reporting standards, the updated shorthand lipid nomenclature, and the organization of ring trials. Second, we would like to initiate a discussion with the attendees to get a feeling of what the lipidomics community would expect from ILS and where ILS still has room for improvement. This discussion can also be regarded as an incentive for the lipidomics community to get involved in ILS and actively shape the future of the research field of lipidomics.

Workshop schedule (75 min)

- M. Holčapek – Introduction & CLIG human plasma lipidome trial (15 min)
- A. Gassiot – Ceramide and bile acids ring trials (15 min)
- J. McDonald – Minimum reporting checklist (15 min)
- Discussion (30 min) - What else can we do for lipidomic community? Suggestions and ideas on how we should do together a better job for the lipidomic community.

TUESDAY WORKSHOPS, 5:45 – 7:00 PM

Tues Workshop 11

Native MS: new approaches to enable discovery in academia and industry

Native Mass Spectrometry Interest Group

Presiding: Justin Benesch, Kristine Parson, Art Laganowsky

General Assembly C

Native MS is recognized as a cutting-edge approach in the molecular characterization of protein targets and therapeutics, and their interactions. It can provide information on assembly stoichiometry, structural integrity, ligand and drug binding, all with unrivalled mass resolution and accuracy. As research targets in academia and industry become more challenging, there is an increasing need to push the limits of native MS in terms of the samples it can address, the ease in which it does so, and how it can integrate with orthogonal technologies.

We are witnessing a continuing growth in native MS and associated methodologies. Exciting developments have been made in the ability to deliver samples of greater inherent complexity, and from "dirty" sources, as well as big steps forward in online delivery and throughput. At the same time, there is continued effort at the interfaces with other MS-based or structural biology methods.

This workshop will highlight the cutting edge of native MS technology development, focusing on disseminating the newest approaches in the field that are breaking down barriers for examining previously intractably complex samples. This workshop, in an informal style, will therefore demystify the state-of-the-art, and be valuable both for newcomers to the individual topics as well as those already proficient in the native MS field.

The native MS workshop has long supported collaboration and knowledge transfer between academia and industry. We are assembling a diverse panel of experts from both theatres; they will each deliver short presentations, and (together with the attendees) participate in an open discussion facilitated by the workshop organisers.

Tues Workshop 12

New fragmentation methods as seen through the lens of radical ion chemistry

Fundamentals Interest Group

Presiding: Yury Tsybin, Alexander Makarov,

Room 340AB

Rapid advances in the resolution and sensitivity of mass spectrometry instrumentation over the last decade have fueled the steady performance enhancement of the arsenal of diverse fragmentation methods. In addition, novel and old ion activation and dissociation reaction ideas have been probed experimentally to further increase the MS/MS capabilities. The most notable recent advances relate to the broader use of higher-energy electrons in, e.g., EID (or EIEIO?) for singly charged small molecule analysis and the combination of multiple fragmentation methods for better characterization of macromolecular complexes.

The dramatic expansion of available data raises the question of whether the established understanding of underlying gas phase ion activation and dissociation chemistry needs any revision - or whether we are already well equipped with our existing models.

This interactive workshop will involve speakers from diverse research areas united by the passion for gas phase radical (and non-radical) ion chemistry and its use to advance the frontiers of analytical science.

They all probably would endorse (and suggest their versions of) the poem composed on the radical ion chemistry theme by ChatGPT:

Radical ions, charged and free,
Soaring high with energy,
In mass spectrometry they dance,
A chemical romance.
With a radical push,
They're torn apart with a rush,
Their masses revealed,
Their secrets to be unsealed.
In the hands of the expert,
This tool never falls short,
Unlocking the mysteries,
Of the world's great histories.

Tues Workshop 13

Non-target analysis (NTA): Modern tools for unknown analysis

Environmental Applications Interest Group

Presiding: Ahmed Hamid, Kevin Tucker

Room 351ABDE

Environmental pollutants cause adverse health effects in humans and ecosystems. Due to rapid industrialization and urbanization, many pollutants have entered the environment, including pharmaceutical compounds, illicit drugs, pesticides, and personal care products. In addition, various per/polyfluoroalkyl substances (PFAS) have been found in many sources such as water, air, fish, soil, food, and food packaging, etc. Interestingly, PFAS degrade very slowly in the environment, which makes them one of the most important research topics for non-target environmental analysis. Liquid chromatography-mass spectrometry (LC-MS) and gas chromatography-mass spectrometry

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(GC-MS) have been used to analyze many pollutants in the environment. Many investigators reported that structural determination of ions can be achieved by high-resolution-MS, ion mobility spectrometry (IMS), and artificial intelligence. For example, one of the artificial intelligence tools is FluoroMatch, which is helpful for automated non-target analysis of PFAS. This workshop will discuss advances and challenges in the analysis of contaminants in the environment by non-target analysis, presented by several scientists in short overviews. This will be followed by a panel discussion led by researchers with relevant experience, along with active engagement of the audience. The goal is to share current experiences and knowledge about different instrumentation platforms for non-target analysis of pollutants in the environment to stimulate further thinking and perspectives among researchers, as well as new artificial intelligence software packages, development of libraries of contaminants, sample preparation, and the benefits of 4D workflows, such as LC-IM-MS/MS.

Tues Workshop 14 **Trans-Proteomic Pipeline: Recent Advances and Future Directions** *Independent*

Presiding: David Shteynberg, Michael Hoopmann
Room 351CF

The workshop will begin with a brief overview of the Trans-Proteomic Pipeline (TPP) and its newest features and capabilities. We will then focus on four individual topics, fostering a discussion with workshop participants on the current strengths, weaknesses, and future directions for the TPP. The workshop will enable participants to describe their challenges in proteomic data analysis and help drive directions in software approaches through needs of the community. The topics for discussion will be focused on the new functionalities in the upcoming TPP version 6.3.0 release, including:

- Overview of the Cloud enabled TPP
- Cleavable crosslinker data analysis with Ving
- Integrating open searching into your usual workflow
- Mining for rare PTMs in your data

Each topic will be introduced with a brief summary of features and ideas. Then feedback and discussion by the workshop participants will be promoted.

Tues Workshop 15 **Imaging MS: Isomer Differentiation in Biological Imaging** *Imaging MS Interest Group*

Presiding: Ingela Lanekoff, Boone Prentice
Room 360ABDE

The differentiation of chemical isomers in mass spectrometry imaging can provide important information on biological processes. However, there are a number of limitations and challenges associated with separating and identifying isomers in conventional biological imaging workflows. A growing number of creative approaches and impressive methods have been reported recently, revealing new levels of chemical detail that provide novel insights into cellular biochemistry. Yet, the almost infinite number of isomeric compounds in biological systems suggests that additional efforts and tools are still required by the community. This workshop aims to discuss the current state of the field and the importance of defining the analyte with isomeric structural resolution. We also seek to highlight promising methods and paths forward that will increase the number of isomers that can be separated in mass spectrometry imaging.

This workshop will be presented in two parts. First, several speakers will briefly describe their methodologies, including the pros and cons, for isomer differentiation in biological imaging. Second, the speakers will serve as a panel for a general discussion with the audience on the challenges that exist within the field, and identify opportunities and strategies for the future. The audience is encouraged to come prepared with questions and ideas.

Tues Workshop 16 **Mass Spectrometry Support for Extractables and Leachables and Biocompatibility testing** *Independent*

Presiding: Gyorgy Vas, Kate Comstock
Room 360CF

Aspects of mass spectrometry support for extractables and leachables for pharmaceuticals and biocompatibility testing for medical devices will be discussed. Discussion will be focused on component identification and the required data support for component identification in the regulated environment. Another discussion topic would be non-targeted testing for biocompatibility, and leachables assessment.

Tues Workshop 17 **Mass Spectral Tools to Enhance Characterization and Identification of Forensic Evidence** *Forensics & Homeland Security Interest Group*

Presiding: Ruth Smith, J. Tyler Davidson
Room 361ABDE

Mass spectrometry is routinely used in forensic science for the characterization and identification of multiple different evidence types, ranging from seized drugs, to explosives, ignitable liquids, trace evidence, and even biological samples. Although GC-MS is perhaps the

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most widely used analytical technique, an increasing number of laboratories are implementing LC-MS/MS and DART-MS systems to enhance workflow and improve sensitivity. Given the continued complexity of forensic evidence submissions, even with these newer techniques, innovative approaches to mass spectral data analysis and data interpretation are needed.

This workshop will include a discussion of current challenges in forensic evidence analysis along with an overview of mass spectral tools developed by the National Institute of Standards and Technology (NIST). The panel will include forensic science practitioners who will discuss challenges within their area of expertise. Representatives from NIST will present various software tools that are freely available (e.g., AMDIS, MS Interpreter) and discuss ways that these tools can be employed to address the identified challenges. After the formal presentations, the moderators will facilitate an open-forum discussion in which workshop participants are encouraged to bring their own challenges for discussion.

WEDNESDAY WORKSHOPS, 5:45 – 7:00 PM

Wed Workshop 01

High throughput screening mass spectrometry - current status and future landscape

Pharmaceuticals Interest Group

Presiding: Kiran Iyer, Jeremy Manheim

Room 310A

High throughput screening (HTS) systems provide the opportunity to measure several hundred thousand samples a day and is therefore in high demand in the pharmaceutical industry. Coupled to a sensitive and specific technique such as mass spectrometry (MS), HTS-MS systems are employed in several stages of the drug discovery process for applications that include, but not limited to, biomarker discovery, disease monitoring, targeted metabolomics, and the development of new chemical entities.

While there are several established MS platforms available for HTS, there are often constraints in trying to balance the throughput and the need for specialized equipment and custom-built software for data analysis. Some common HTS-MS platforms include the RapidFire-MS, multiplexed LC-MS/MS systems, Acoustic systems coupled to MS, MALDI-MS, and the more recently emerging HTS-DESI-MS systems.

This workshop aims to present:

- 1) The status on the use of HTS-MS systems for pharmaceutical analysis
- 2) Current developments, instrumentation, limitations and constraints with HTS-MS systems
- 3) Future outlook

The workshops aims to gather several presenters from instrumentation and pharmaceutical companies. Order of the presentations will be: 1) opening remarks from the presiders covering Topic 1, 2) two presentations from instrument companies (Bruker, Sciex) 3) two presentations from scientists in the pharmaceutical industry, and 4) closing remarks by the presiders.

The audience for the workshop will be the industry community, researchers in academia, and analytical contract laboratories. Appropriate time will be designated to encourage participation and idea exchange with the audience. An expected outcome is to trigger the interest in the industry to embrace HTS-MS and for instrument companies to showcase exciting developments within this space.

Wed Workshop 02

Late-Night Lightning Lectures!

Independent

Presiding: Emily Sekera

Room 310BC

This workshop will provide poster presenters a chance to present a 90-second lightning talk consisting of one slide maximum. This activity is intended to help challenge presenters to put their knowledge-translation skills to the test and gain experience presenting at a podium. It is our hope that the lightning talk will help speakers to garner interest in their posters during the week. Speakers will be chosen before the conference that cover a wide range of topics within ASMS. After the announcement of oral and poster presenters and confirmation of the workshop, we will send out a survey to aid in finding scientists interested in presenting. Preference will be given to speakers in labs who do not have an oral presentation at ASMS Houston 2023. Time permitting and level of interest, we will either conclude with a 15-minute open forum to allow audience members to give feedback to presenters and ask questions.

Wed Workshop 03

Utilizing GC/MS Technologies and Associated Software Tools to Address Challenging Applications in the Flavor, Fragrance and Foodstuffs Laboratory

Flavors, Fragrance, and Foodstuff (FFF) Interest Group

Presiding: Joe Binkley, Liz Humston-Fulmer

Room 320A

There are many challenging questions that a flavor, fragrance or food laboratory may be tasked to answer. These applications can include developing new products, reformulating competitive products, creating effective quality control methodologies, or identifying off odors and flavors, among many others. Addressing these challenges generally requires both hardware and software solutions. Due to the nature of many of the molecules responsible for a product's flavor and fragrance profile, GC/MS is frequently the hardware tool of choice. Once samples are analyzed, gleaning useful information from the rich GC-MS data is the next analytical challenge. Software tools that automate data processing and compile analyte information from the various samples can facilitate data review and improve efficiency for analytical scientists in this application field.

The goal of this workshop is to enhance attendees' knowledge about software tools which are available to make their day-to-day tasks easier and more efficient. Some of the software attributes which will be demonstrated during this workshop will include automated peak finding/identification, comparison strategies, and strategies for processing and comparing groups of samples. These demonstrations will serve as a starting point for a group discussion intended to engage and benefit attendees.

The workshop format will consist of two parts: 1) Panelists will provide brief examples and demonstrations of software tools which were used to effectively extract information from analytical data to solve real world problems in their laboratories. 2) Interactive discussion among attendees and panelists moderated by the interest group coordinators, including engagement with attendees by interactive, smartphone-based polling.

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Wed Workshop 04 Biomarkers Development: How Mass Spectrometry Is Changing the Field *Regulated Bioanalysis Interest Group*

Presiding: Wenkui Li, Jian Wang
Room 320BC

A biomarker or biological marker is considered a measurable indicator of a certain biological state or disease related condition. Biomarkers are often evaluated qualitatively or quantitatively using blood, urine or tissues to examine normal biological processes, pathogenic processes, or pharmacologic responses to a therapeutic intervention. LC-MS is a powerful analytical tool for the analysis of various biomarkers including small molecule and large molecule biomarkers. This workshop is to be featured by presentations covering LC-MS biomarker analysis- 'When? How? Why? hybrid LC-MS for protein biomarker quantitation, use of a universal surrogate matrix assay for biomarker analysis, and quantitative target occupancy analysis using immunoaffinity capture 2D-LC-MS/MS, etc.

This workshop will develop future discussions and consensus on LC-MS biomarker analysis in support of regulated studies, including topics on sample preparation, mass spectrometric methods and data processing. Experts in the field will share their experience in this highly interactive workshop.

Wed Workshop 05 Ion Mobility Spectrometry: From Data to Structure *Ion Mobility MS Interest Group*

Presiding: James Prell, Xueyun Zheng
Ballroom A

In addition to separating isobaric analyte ions and increasing peak capacity, Ion Mobility (IM) Spectrometry can often help characterize ion structure. However, the drift time/collision cross section (CCS)-ion structure relationship can be complicated, whether in predicting a CCS from a model structure or vice versa. State-of-the-art methods for these tasks range from using detailed physical modeling of the ion-gas scattering process to using Machine Learning based on molecular descriptors and experimental CCS databases. These methods differ in their emphasis on the parent condensed-phase structure versus structure after transfer into the gas-phase environment. This workshop aims to stimulate discussion about the advantages and challenges of a range of strategies for structural interpretation of IM-MS data. After a brief (5 minute) introduction to the problem of relating IM-MS data to ion structure by the presiders, we will feature perspectives spanning industry and academic research, as well as empirical versus first-principles approaches. We aim to invite a panel of speakers that are working on different approaches, such as conventional "frozen-structure" scattering models, Machine Learning/molecular descriptor-based approaches, and molecular dynamics approaches. Example topics of discussion include: When might it be useful to understand the structures of gas-phase ions, if they have changed significantly from those in the condensed phase? Should we focus in the future on more accurate scattering models or on improving predictive capabilities of molecular descriptors? How can these approaches learn from each other?

Wed Workshop 06 MS Career Options: How to Kick Start Your Career *Young Mass Spectrometrists Interest Group*

Presiding: Christopher Pulliam, Ryan Bain
Ballroom B

Description: The Young Mass Spectrometrists workshop focuses on a panel discussion where representatives of various careers paths discuss their journey to their current position and answer questions regarding their current and past experiences. Through this discussion mass spectrometrists at the undergrad, graduate, or postdoctoral stage of their career learn information or strategies that will help them navigate the next steps in their career. This panel typically comprises representatives from a wide swath including academia, biotech/pharma, start-up companies, government, and non-traditional career paths to provide a comprehensive view of career opportunities for young researchers who have mass spectrometry skills.

Wed Workshop 07 Ambient Ionization in Application Fields: What is Required, Desired, and Provided? *Ambient Sampling & Ionization Interest Group*

Presiding: Chris Gill, Roshan Javanshad, Jacob Jordan
Ballroom C

Ambient ionization mass spectrometry has been a durable topic at ASMS since 2006 ("Direct Ionization Techniques"). Since the first workshop in 2019, it has been a great platform for attendees to discuss innovations and issues in instrumentation, sampling, ionization, and related applications, as well as the underlying scientific mechanisms. In recent years (2021, 22), this workshop had 50 and 86 attendees from academia, industry, and government. At the first workshop in 2019, concerns and interest in the field were polled from some 200 attendees. The workshops in the following years have responded to the interests of our community, with foci of "reproducibility, 2020", "quantitation, 2021", and "molecular coverage, 2022".

This year, the workshop will highlight the applications of ambient ionization while continuing our discussion of these figure of merit (FoM) topics. The versatility of ambient ionization methods makes mass spectrometry approaches more accessible in a wide range of areas including forensics, security, environmental analysis, manufacturing, imaging, and clinical/point-of-care diagnostics. Each application has a set of different desired and required FoMs for analytical methods. Besides exhibiting the state of the art in these areas via lightning talks, the workshop will survey these FoMs in relevant applications. Attendees will put stickers on a prepared poster (like in 2019) to

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indicate the desired FoMs (sensitivity, accuracy, molecular, etc.) in their application/areas. Expert panelists will lead a Q&A-style discussion that covers challenging aspects, recent breakthroughs, and potential research directions in our research community.

Wed Workshop 08 **Target Protein Degradation and MS-based Proteomics** *Independent*

Presiding: Pankaj Dwivedi
Room 3332

Target Protein Degradation (TPD) research field is evolving rapidly. Given proteins are the functional unit of the cell, it is very promising to target "bad" proteins in the cell with respect to finding a potential therapeutic avenue for certain disease. Proteomics has always been instrumental in understanding of the normal and disease biology. This workshop is dedicated to understanding/ active discussion regarding the opportunities and challenges associated to MS-based proteomics for TPD.

Wed Workshop 09 **What are the future needs of photoionization mass spectrometry for complex mixture analysis?** *Photoionization MS*

Presiding: Christopher Rürger
General Assembly A

Photoionization schemes for mass spectrometry, either by laser or discharge lamps, have been widely examined and deployed for almost every application area and field of science. Fundamentals on the reaction mechanisms for atmospheric pressure photoionization (APPI) have been described in the early 2000s. Different manufacturers developed and launched APPI sources commercially, and various research groups published on specific geometries and designs. However, APPI development has been largely halted, and APPI has fallen into a niche without major commercialization. Consequently, this workshop aims to address the future needs for APPI development and potential application areas in complex mixture characterization from the fields of environmental and material sciences as well as energy transition. Questions are raised for: What are the light sources utilized in the mass spectrometry market for photoionization? What novel light sources are available and might be handy in mass spectrometry, such as innovative laser concepts, e.g., OPO? What are photoionization's unique chemical application fields and benefits, and how can this be combined with established ESI/APCI workflows? The workshop will feature different short presentations to initiate a discussion atmosphere.

Wed Workshop 10 **Houston, We Have a Microbiome Problem (...and how the Metaproteomics Initiative aims to solve it!)** *Independent*

Presiding: Pratik Jagtap, Robert Hettich, Timothy Griffin, Tim Van Den Bossche
General Assembly B

Mass spectrometry-based metaproteomics research has experienced rapid growth due to its ability to help characterize complex microbial communities and is likely to become a central approach for understanding how microbiomes function. Despite its value, metaproteomics offers analytical and bioinformatic challenges beyond those encountered in traditional, single-organism MS-based proteomics. As a solution, the Metaproteomics Initiative (www.metaproteomics.org) is a global initiative that promotes the dissemination of metaproteomics fundamentals, analytical and bioinformatic advancements, and microbiome applications. Members of the Initiative will present the updates on two recent CAMPI (Critical Assessment of Metaproteome Investigation) benchmark studies on sample preparation and functional annotations, and future projects that will be designed to propel this field forward. The members will also provide highlights from the 5th International Metaproteomics Symposium (Avignon, France), which was held in April 2023.

The workshop will invite a panel of leading metaproteomics experts who will participate in a discussion that covers the status of metaproteomics, research needs, and growth opportunities. The panel will also interact with the audience and address discussion points on how the initiative will help in gaining deeper insights into microbiome dynamics. The workshop will also describe the Initiative along with information on how interested researchers can join, participate, and contribute to its growth.

Wed Workshop 11 **Hispanics and Latinx in Mass Spectrometry** *Independent*

Presiding: Benjamin Garcia, Livia Eberlin, Francisco Fernandez Lima
General Assembly C

This workshop proposal looks to organize the first official meeting of the newly forming Hispanics and Latinx in Mass Spectrometry outside interest group. Since 2003, Hispanics/Latinx have been one of the largest growing minority groups in the United States population. Nevertheless, this has not been reflected in our ASMS community membership of scientists. According to the ASMS demographic data, Hispanics/Latinx only comprise ~3% of the scientist membership, well under the U.S. population average. In order to continue to support and grow this important group, several Hispanic/Latinx scientists have come together to begin to form a new outside interest group. It is our hope that by becoming more visible and active at ASMS Conferences and beyond, we can encourage the younger Hispanic/Latinx scientists to become more involved in the mass spectrometry field. Specifically for this workshop at the ASMS Conference, we plan to have an event where we will showcase the research that Hispanic/Latinx scientists are currently engaging in, making sure to highlight the younger members of our society. It is hoped that in addition to the cutting-edge research, the speakers will also discuss their personal journeys that got them to this point in their careers. Additionally, we'd like to spend some time to have an open panel discussion to give the opportunity to our audience to ask questions, and also to solicit ideas and feedback on how this new outside interest group can be

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more effective to organize, outreach and grow. It is anticipated that this workshop will be the first event catalyst to encourage and support the Hispanic/Latinx members of ASMS. This workshop is open to anyone who identifies as Hispanic/Latinx in any way, and also to members who have trainees/co-workers from these groups as well (Allies).

Wed Workshop 12
Polymeric materials: tackling hydrocarbon-based polymers
Polymeric Materials Interest Group
Presiding: Thierry Fouquet, Anthony Gies
Room 340AB

Following a brief introduction on the interest group business (application for Sanibel/Asilomar conference, informal meetings), we will start out discussing the analysis of hydrocarbon polymers with one presentation from a member (10-15 min). The presentation will include a brief overview of existing MS techniques for the microstructure analysis of styrenic and olefinic polymers and cover the current limitations / possible solutions to explore. Attendees are invited to ask questions throughout the presentation. The main part of the workshop will then take the form of a live session of data processing using commercial and free programs for the exploration of complex MS and MS/MS data. The hosts (one or both organizers, at least one more invited presenter) will provide examples to show the advantages of advanced data analysis approaches. Attendees are encouraged to share their own datafiles in advance - or during the workshop to spice up the demonstration - to help drive the interactivity. Such a live demonstration (at least 40 min) will be the first of its kind for our interest group and will undoubtedly trigger fruitful discussions among members. It is envisioned that the flow of ideas will enable the development of new data analysis tools or pinpoint the need to modify preexisting software solutions. The final discussion (typically 15 minutes) will be focused on the potential use of ion mobility to complement MS for the detailed characterization of these highly complex polymeric materials (tentative topic), and/or any topic attendees may wish to tackle, e.g. via the presentation of a single slide of their results/ideas.

Wed Workshop 13
ProteomicsML: An online educational platform for machine learning in proteomics
Independent
Presiding: Juan Antonio Vizcaíno
Room 351ABDE

Open data science practices in proteomics have been largely driven by the efforts of the Proteomics Standards Initiative (PSI, <http://www.psidev.info>) and the ProteomeXchange Consortium of proteomics resources (<http://www.proteomexchange.org>). Both are two highly collaborative community initiatives that are open to the contribution and ideas from everyone. Since 2002, the mission of the PSI is the development and promotion of open data standards and related software in the proteomics field. Some recent and ongoing projects are focused on the development of a standard format for spectral libraries (mzSpecLib), the standard notation ProForma 2.0 for peptidoforms and proteoforms and the Universal Spectrum Identifiers, apart from updates in other widely adopted formats such as mzML and mzIdentML. In a parallel effort, since 2012, the ProteomeXchange Consortium is standardising the submission and dissemination of public proteomics data between the main proteomics data repositories, currently including the resources PRIDE, PeptideAtlas, MassIVE, jPOST, iProx and Panorama Public.

We will briefly highlight current trends in the increasing re-use of public proteomics datasets. As a key recent output of open science practices in the field, we will highlight the ProteomicsML platform (<https://proteomicsml.org/>). ProteomicsML provides ready-made datasets for machine learning models accompanied by tutorials on how to work with even the most complex data types. The resource is set up to evolve together with the field, and we welcome everyone to contribute to the project by adding new datasets and accompanying notebooks.

Wed Workshop 14
Art, Museums, and Archaeology
Independent
Presiding: G. Asher Newsome, Paul A. Haynes
Room 351CF

The study of artworks, archaeological specimens, and other cultural heritage objects by mass spectrometry requires the adaptation of previously developed techniques, as well as the development of new approaches. Analytical methods used in biomedicine, industrial and natural product research, and forensics must be carefully tailored to be successfully applied in diverse fields such as anthropology, archaeology, natural history, art history, paleontology, and more. This multidisciplinary workshop will feature lightning talks selected from ASMS poster abstracts - students and fellows are encouraged to volunteer in advance by contacting the organizers. Lightning talks will be followed by audience Q&A with a panel of academic, government, and private institution scientists to discuss areas of interest in the field. This will provide a great opportunity to exchange detailed information about essential methodology which is often excluded from published literature. Science and science-adjacent topics may include: ethics and permissions involved in analyzing culturally sensitive samples; the risk of damage to objects as a result of analysis; sample-limited preparation and recovery approaches for rare and precious analytes; considerations for historical and contemporary sample contamination; the significance of preservation and prediction of material degradation; discerning the importance of chemicals identified from an analyte removed from context; employment, funding, and fellowship opportunities; and many more.

WEDNESDAY WORKSHOPS, 5:45 – 7:00 PM

Wed Workshop 15

Remote Sample Collection and Microsampling is Driving New Mass Spectrometry Analytical Solutions *Independent*

Presiding: Donald Chace, Timothy Garrett

Room 360ABDE

Large volumes of blood, urine and other biological fluids (1mL or more) are becoming more obsolete and impractical in clinical chemistry practice with the exception of the inpatient environment (hospital). There is a shift in demand for sampling outside of the hospital or clinic because of concerns regarding access, rise in telemedicine, and the desire for direct to patient solutions. The covid pandemic likely accelerated this sea change in biological fluid sampling.

Remote sampling of biological fluids relies on volumes that are much smaller roughly defined as less than 1 ml and typically is in the range of 50- 300 uL needed on average during collection. This microsample can be either liquid (wet) or a dried in a matrix such as paper. Newborn screening has used the dried microsample for more than 50 years as part of its sample collection format from newborns. The analysis of these DBS includes many classical clinical chemistry methods as well as mass spectrometry (specifically tandem MS). There are many issues facing microsampling in terms of precision and accuracy of such small volumes whether they are wet or dry. For mass spec, an inherently selective and accurate measurement device, precision is important as well as detection limits, limits of quantification etc. Further automation of sampling handling, interpretation are all issues that are important, many of which were identified in newborn screening. Microsampling has numerous advantages but also challenges that are being addressed.

This interest group will be focused on best practice for microsampling from isotope dilution MS, standardization, recovery from the matrix, analyte stability, suitability for analysis. It is a rapidly evolving field for which mass spec is a key player from small molecule to proteins. Cost and convenience is a huge driver of this technology as well and this group should attract a good attendance.

Wed Workshop 16

Knowledge Share and Instrumentation Donations for Developing World Outreach *Developing World Outreach Interest Group*

Presiding: Giles Edwards, Kym Faulk

Room 360CF

This new ASMS Special Interest Group (SIG) aspires to bring together those who wish to share their ideas on how we as a society can assist in deploying mass spectrometry as a key analytical technique to address educational, health, environmental and economic issues in the Developing World. The idea to establish this SIG stemmed from workshops entitled "Mass Spectrometry in the Developing World: supporting education and research", held for the past three years at the annual ASMS meetings. Future correspondence will address the items on the agenda to be addressed. For now, we invite all interested ASMS members to join the SIG and follow the postings on this site.

The organizing committee of this group have shipped and installed a number of mass spectrometry products in developing countries for academia. If any ASMS members would like to contribute redundant instrumentation, their engineering or applications based knowledge it would be gratefully received. The group aims to work out a strategy to utilize the skill set of ASMS members for outreach activities.

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

Art, Archaeology & Paleontology	001-009
Biomarkers: Discovery I	010-035
Biomarkers: Quantitative Analysis I	036-060
Biomolecular Structure Analysis:	
Chemical Crosslinking and	
Covalent Labeling	061-079
Cancer Research I	080-106
Clinical Analysis I	107-131
Covalent Labeling and Chemical Crosslinking I	132-150
Disease Biomarkers	151-171
Drug Discovery: Qualitative	
and Quantitative Analysis I	172-191
Epigenetic Modifications	192-201
Food Safety: General	202-230
Fundamentals: Ion Molecule, Ion/Ion,	
Ion/Electron Interactions	231-248
Fundamentals: Native MS	249-268
Glycoproteins I	269-293
High Throughput MS I	294-316
Imaging MS: Computational Methods, Software,	
and Analysis	317-335
Imaging MS: Method Development I	336-364
Informatics: Algorithms and Statistical Advances	365-392
Instrumentation: General	393-411
Ion Mobility: FAIMS/DMS	412-420
LC/MS: Sample Preparation I	421-438
Lipids: General	439-466
MALDI: Applications	467-479
MALDI: Innovation in Instrumentation	
and Sample Preparation	480-492
Metabolomics: Clinical Applications	493-504
Metabolomics: Sample Preparation	505-511
Microorganisms and the Microbiome	512-543
Nanoscale and Microfluidic Separations and MS	544-551
Peptidomics	552-569
Phosphopeptides and phosphoproteins	570-588
Plant Biology and Biotechnology	589-602
Protein Therapeutics: Structural Characterization	603-630
Proteins: Conformation Analysis	
and Structural Biology	631-662
Proteins: PTMs I	663-687
Proteomics: Infectious Diseases	688-701
Proteomics: Intact Proteins and Top Down Analysis I	702-721
Proteomics: Quantitative I	722-741

- MP 001 **Developing a molecular approach to the species identification of plant-based fibres in ancient Egyptian textiles using mass spectrometry;** Dylan H Multari¹; Michelle F Whitford¹; Ronika K Power¹; Paul A Haynes¹; ¹Macquarie University, Sydney, Australia
- MP 002 **Metabolomics on osteoarchaeological material allows the discovery of biomarkers related to the consumption of tobacco in ancient British populations;** Diego Armando Badillo-Sanchez¹; Maria Serrano Ruber¹; Anna M. Davies-Barret¹; Donald J. L. Jones¹; Sarah A. Inskip¹; ¹University of Leicester, Leicester, United Kingdom
- MP 003 **Sex determination of four two-million-year-old Paranthropus robustus fossil teeth from South Africa by mass spectrometry;** Claire Koenig¹; Palesa Petunia Madupe¹; Ioannis Patramanis¹; Patrick L. R  ther¹; Nomawethu Hlazo²; Meaghan Mackie^{1,3}; Lauren Schroeder⁴; Alberto John Taurozzi¹; Cl  ment Zanolli⁵; Fernando Racimo¹; Jesper Velgaard Olsen¹; Rebecca Rogers Ackermann²; Enrico Cappellini¹; ¹University of Copenhagen, Copenhagen, Denmark; ²University of Cape Town, Cape Town, South Africa; ³University College Dublin, Belfield, Ireland; ⁴University of Toronto, Toronto, ON; ⁵Universit   de Bordeaux, Bordeaux, France
- MP 004 **MALDI MS, ATR/FTIR & Raman Imaging - a Comprehensive Toolbox to Assess Environmental Damage in Cultural Parchment Objects;** Antonia Malissa^{1,2}; Manfred Schreiner^{1,2}; Martina Marchetti-Deschmann¹; ¹TU Wien, Vienna, Austria; ²Academy of Fine Arts Vienna, Vienna, Austria
- MP 005 **Insights into patterns and pathways of protein degradation: A case study with   -lactoglobulin;** Bharath Nair¹; Meaghan Mackie²; Tina Ravnsborg³; Samantha Presslee⁴; Kirsty Penkman⁴; Jesper Velgaard Olsen¹; Ole Jensen³; Carsten Wiuf¹; Matthew Collins^{1,5}; ¹University of Copenhagen, Copenhagen, Denmark; ²University College Dublin, Belfield, Ireland; ³University of Southern Denmark, Odense, Denmark; ⁴University of York, Heslington, United Kingdom; ⁵University of Cambridge, Cambridge, United Kingdom
- MP 006 **New perspectives in archaeological textiles: a unique workflow for the double characterization of dyes and proteins from extremely degraded relics;** Iaria Serafini^{1,2}; Gabriele Favero¹; Roberta Curini¹; Gw  na  lle M. Kavich²; Timothy P. Cleland²; Caroline Solazzo²; ¹Sapienza University of Rome, Rome, Italy; ²Smithsonian Museum Conservation Institute, Suitland, MD
- MP 007 **Chromatography-free analysis of pigments by high resolution mass spectrometry with direct sample introduction;** Sam Putnam¹; Rachel Lackner²; William L. Fatigante¹; Nobuko Shibayama²; Maria Goretti Mieites Alonso²; ¹Bruker Scientific, LLC, Billerica, MA; ²The Metropolitan Museum of Art, New York City, NY
- MP 008 **Comparing Intramineral proteins from the eggshells of ratite birds, crocodiles and a dinosaur eggshell fossil;** Connor E. Gould¹; Rocio Elejalde Cadena²; Alan Friedman³; Abel Moreno²; Troy D. Wood¹; ¹Department of Chemistry, University at Buffalo, Buffalo, NY; ²Instituto de Qu  mica, Universidad Nacional Aut  noma de M  xico, Ciudad de M  xico, Mexico; ³Department of Materials Design and Innovation, School of Engineering and Applied Sciences, University at Buffalo, Buffalo, NY
- MP 009 **Collagen Remains in Palaeotherium Bone from the Isle of Wight (UK);** Joseph Hubbard¹; Steven Robinson²; Arden Hulme-Beaman³; Martin Munt⁴; Krzysztof Pawlak²; Steve Taylor¹; ¹Department of Electrical Engineering & Electronics, University of Liverpool, Liverpool, United Kingdom; ²Materials Innovation Factory, University of Liverpool, Liverpool, United Kingdom; ³University of Liverpool, Liverpool, United Kingdom; ⁴Dinosaur Isle Museum, Sandown, United Kingdom
- MP 010 **The First Profile of Steroid Hormones in Human Aqueous Humor is Generated from the LC MS/MS Approach;** Tiansheng Chou^{1,2}; Xiaosheng Huang³; Jun

MONDAY POSTERS

- Zhao^{3,4}; Siqi Liu⁵; ¹BGI, Shenzhen, China; ²College of Life Sciences, University of Chinese Academy of Sciences, Beijing, China; ³Shenzhen Eye Institute, Shenzhen Eye Hospital, Jinan University, Shenzhen, China; ⁴Department of Ophthalmology, Shenzhen People's Hospital (The Second Clinical Medical College, Jinan University; The First Affiliated Hospital, Southern University of Science and Technology), Shenzhen, China; ⁵BGI, Shenzhen, China
- MP 011 **Direct measurement of Plasma Phosphatidylinositols and Polyphosphoinositides in Lung Cancer Patients Using UHPLC/MS/MS;** Hai Bui¹; Kenneth D. Roth¹; ¹Eli Lilly and Company, Indianapolis, IN
- MP 012 **Structural proteomic profiling of cerebrospinal fluids to reveal novel conformational biomarkers for Alzheimer's disease;** Bin Wang¹; Xiaofang Zhong¹; Lauren Fields¹; Haiyan Lu¹; Zexin Zhu¹; Lingjun Li¹; ¹UW-Madison, Madison, WI
- MP 013 **High salt diet damaged blood vessel and induced hypertension is elucidated by vascular bed systematic profiling;** Siu Kwan Sze; Brock University, St Catharines, ON
- MP 014 **High-performance metabolic fingerprints of aqueous humor for retinoblastoma monitoring;** Wanshan Liu¹; Kun Qian²; ¹Shanghai Jiao Tong University, Shanghai, China; ²Shanghai Jiao Tong University, Shanghai, China
- MP 015 **Proteomics Analysis of Rheumatoid Arthritis Patients' sera Identifies Multi-Biomarker for Predicting Infiximab Response;** Ara Cho¹; Jinsung Ahn¹; Andrew Kim¹; Eugene C. Yi¹; ¹Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology and College of Medicine or College of Pharmacy, Seoul National University, Seoul, South Korea
- MP 016 **Tear metabolic fingerprinting identifies glaucoma;** Jiao Wu¹; Kun Qian²; ¹Med-X Research Institution, SJTU, Shanghai, China; ²Shanghai Jiao Tong University, Shanghai, China
- MP 017 **Metabolomic Profiling of Cancer Biomarkers from Methanol Extracts from Pathology Specimens using LC-MS/MS;** Alexandra M. Izydorczak¹; Wilfrido D. Mojica¹; Troy D. Wood¹; ¹SUNY at Buffalo, Buffalo, NY
- MP 018 **Contribution of the microbiome to a metabolomic signature predictive of risk for pancreatic cancer;** Johannes Fahrman¹; Ehsan Irajizad²; Jody Vykoukal²; Ranran Wu²; Jennifer B Dennison²; James P Long²; Anirban Maitra²; Kim-Anh Do²; Samir Hanash²; ¹University of Texas, MD Anderson, Houston, TX; ²UTMDACC, Houston, TX
- MP 019 **Novel LC-MS Strategies to Enable Discovery and Quantification of Gluten Immunogenic Peptides and Their Deamidated Forms in Human Urine;** Jie Pu¹; Qingqing Shen¹; Chao Xue¹; Timothy Sikorski²; Thomas Angel²; Zhuo Chen²; John T Mehl²; Huaping Tang²; Jun Qu^{1,3}; ¹University at Buffalo, Buffalo, NY; ²GSK, Collegeville, PA; ³New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY
- MP 020 **Study of the cholesterol biosynthesis pathway perturbation in demyelination/remyelination of cuprizone mice using GCMS and proteomics;** Xiaoping L Hronowski¹; Rongfang Gu¹; Kayla Soucey¹; Benbo Gao¹; Zhaohui Shao¹; Ru Wei¹; ¹Biogen, Cambridge, MA
- MP 021 **Biomarker discovery pipeline with chemical isotope labeling LC-MS method;** Wayne Cheng¹; Rui Qin¹; Shuang Zhao¹; Liang Li^{1,2}; ¹The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta; ²University of Alberta, Edmonton, AB
- MP 022 **Depleted or non-depleted serum, establishing a best practice approach for monitoring peptide biomarkers using DIA methodologies;** Alison Porter¹; Abigail Burrows Franco¹; Cecily R Wood¹; Scott M Peterman²; Scott D Stanley¹; ¹University of Kentucky, Lexington, KY; ²Thermo Fisher Scientific, San Jose, CA
- MP 023 **Biomarker discovery in human plasma samples from patients suffering from myalgic encephalomyelitis and post-viral fatigue using mass spectrometry-based quantitative proteomics;** Ganna Shevchenko¹; Anastasiya Ushenkina¹; Jonas Bergquist^{1,2}; ¹Department of Chemistry - Biomedical Center, Analytical Chemistry and Neurochemistry, Uppsala University, Uppsala, Sweden; ²The ME/CFS Research Centre, Uppsala University, Uppsala, Sweden, Uppsala, Sweden
- MP 024 **DIA-MS-based proteomics for discovery of protein biomarker signature from >100 cancer plasma samples;** Yi-Ju Chen¹; Kuen-Tyng Lin¹; Yi-Jing Hsiao²; Gee-Chen Chang³; Jin-Shing Chen⁴; Sung-Liang Yu²; Yu-Ju Chen¹; ¹Institute of Chemistry, Academia Sinica, Taipei, Taiwan; ²Department of Clinical Laboratory Sciences and Medical Biotechnology, College of Medicine, National Taiwan University, Taipei, Taiwan; ³Institute of Medicine of Chung Shan Medical University, Taichung City, Taiwan; ⁴Department of Surgical Oncology, National Taiwan University Cancer Center, Taipei, Taiwan
- MP 025 **Development of a Biomarker Discovery Pipeline for High-Grade Serous Carcinoma using Biofluid Extracellular Vesicles and Data-Independent Acquisition;** Tyler T. Cooper^{1,2}; Lynne M Postovit¹; Gilles A Lajoie²; ¹Queen's University, Kingston, ON; ²Western University, London, ON
- MP 026 **Improved Quantitative Approach for Monitorization of Gangliosides Structural Diversity in Fungal Cell Factories by LC-MS/MS;** Javier Fernando Montero-Bullón¹; Javier Martin-González¹; Gloria Muñoz-Fernández¹; Alberto Jiménez¹; Jose Luis Revuelta Doval¹; ¹University of Salamanca, Salamanca, Spain
- MP 027 **Sample preparation using dried blood devices enables quantification of 3900 proteins from whole blood and biomarker identification in lung cancer;** Natasha Lucas¹; Cameron Hill¹; Elisabeth Karsten¹; Dana Pascovici²; Rosalee McMahon¹; Ben Herbert¹; ¹Sanguis Bio, Sydney, Australia; ²Insight Stats, Sydney, Australia
- MP 028 **Proteomic evaluation of sex differences in the plasma of non-human primates exposed to ionizing radiation for biomarker discovery;** Christina Williams¹; Mehari Weldemariam¹; Maureen A. Kane¹; ¹University of Maryland, School of Pharmacy, Baltimore, MD
- MP 029 **LC-MS based translational pharmacoproteomics allows the discovery of drug-perturbed liquid biomarkers across species bridging preclinical and clinical biomarker decision-making strategies;** Andreas David Brunner¹; Anouk Oldenburger¹; Larissa Pfisterer¹; Daniel Veyel¹; Eva Griesser¹; Wolfgang Rist¹; Patrycja Schlingeloff²; Julian Schmidberger²; Mark Haenle²; Wolfgang Kratzer²; Heike Neubauer¹; Markus Werner¹; Tom Bretschneider¹; ¹Boehringer Ingelheim Pharma, Biberach, Germany; ²Department of Internal Medicine I, University Hospital Ulm, Ulm, Germany
- MP 030 **Development of red blood cells and plasma-based diagnostic lipid biomarker panel for Parkinson's disease;** Fathima Shaima Muhammednazaar¹; Anne M Roberts¹; Ankit Jain¹; Malcolm Horne²; Stephan Klatt³; Blaine Roberts¹; ¹Emory School of Medicine, Emory University, Atlanta, GA; ²CSIRO Health and Biosecurity, Herston, Australia; ³Institute for Vascular Signaling, University of Frankfurt-Goethe University, Germany
- MP 031 **Unbiased Biomarker Discovery for IBD Target Validation and Patient Stratification;** Mostafa J Khan¹; Faizan Zubair¹; Chris Deboever¹; Paul Harris¹; ¹Takeda Pharmaceuticals, San Diego, CA
- MP 032 **Exploration towards the novel biomarkers of human cystic echinococcosis based on coupling of LC-MS/MS and immunoassay;** Congmin Zhang¹; Xi Gao^{1,2}; San A¹; Sang Hua¹; Wangmu Danzeng¹; Jin Zi¹; Siqi Liu^{1,2}; ¹Beijing Genomics Institute, shenzhen, China; ²College of Life Sciences, University of Chinese Academy of Sciences, Beijing, China

MONDAY POSTERS

- MP 033 **Development of proteomic biomarker panel for Cervical Cancer from Indian population;** Amrita Mukherjee¹; Sanjeeva Srivastava¹; ¹*IIT Bombay, Mumbai, India*
- MP 034 **A Comprehensive Strategy for Building and Evaluating Plasma Proteomics DDA Derived Spectral Libraries with ZENO-TOF 7600;** Yi (Jimmy) Zeng¹; Hao Qian¹; Ruby Karimjee¹; Joon-Yong Lee¹; Mark Marispini¹; Jessica Chan¹; Megan Mora¹; Benjamin Ta¹; Ehdieh Khaledian¹; Chi-Hung Lin¹; Robert Zawada¹; Philip Ma¹; Bruce Wilcox¹; ¹*PrognomiQ Inc, San Mateo, CA*
- MP 035 **Optimization of a multi-omic workflow for biomarker discovery in a medaka fish model of chronic low dose ionizing radiation exposure;** Sydney Bedillion¹; Michael Tiemeyer¹; Franklin E. Leach III¹; ¹*University of Georgia, Athens, GA*
- MP 036 **Quantitative reagent-free bioanalysis of proteins in humanized mouse models: Enrichment and Normalization Strategies;** Jinqing Deng¹; Eugene Ciccimaro¹; Petia Shipkova¹; ¹*BMS, Princeton, NJ*
- MP 037 **Liquid chromatography-tandem mass spectrometry reveals association of acute myocardial infarction risk with the dynamic balance between trimethylamine-N-oxide, betaine, and choline;** Sam Li¹; Shan Huang^{1,2}; Si Ying Lim¹; Sock Hwee Tan¹; Mark Chan¹; Wuzhong Ni²; ¹*National University of Singapore, Singapore, Singapore;* ²*Zhejiang University, Hangzhou, China*
- MP 038 **Development and Validation of the Measurement of Cotinine and Hydroxycotinine in Serum: An Automated Sample Preparation and new LC/MS/MS Method;** Danielle L Sowle¹; Tiffany H Seyler¹; Madeline L Weaver¹; Lanqing Wang¹; ¹*CDC, Atlanta, Georgia*
- MP 039 **Deep Proteomic Profiling of the Serum Proteome Across the Murine Lifespan;** Amit K Dey¹; Simonetta Camandola¹; Nathan L Price¹; Slam Investigators¹; Rafael de Cabo¹; Nathan Basisty¹; ¹*National Institute on Aging-NIH, Baltimore, MD*
- MP 040 **A path from discovery to targeted proteomics approach for the verification and validation of tissue-derived biomarkers in coronary artery diseases;** Chi D. L. Nguyen¹; Jonathan Bui¹; Zachary Dwight¹; Jesse G. Meyer²; Austin L. Seal³; Annie Moradian¹; Stephen A. Whelan¹; Mitra Mastali²; Sarah J. Parker²; David M. Herrington³; Susan Mockus¹; Jennifer E. Van Eyk²; ¹*Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA;* ²*Heart Institute & Advanced Clinical Biosystems Research Institute, Los Angeles, CA;* ³*Department of Cardiovascular Medicine, Wake Forest University, Winston-Salem, NC*
- MP 041 **A Rapid Method for Simultaneous Quantification of Monoamines in Rat Brain in a Tetrabenazine-Induced Model of Depression;** Lilia Magomedova¹; Sophie R Pan¹; Julia Izhakova¹; Monica Ortiz¹; Guy A Higgins²; Leo B Silenieks²; Ines De Lannoy¹; ¹*Transpharmation Canada Ltd, Mississauga, ON;* ²*Transpharmation Canada Ltd, Fergus, Ontario*
- MP 042 **A targeted workflow for investigating the tear proteome of patient with Sjogren's syndrome by LC-MS/MS;** Maggie Lepine¹; Marie-Claude Robert^{2,3}; Lekha Sleno^{1,3}; ¹*University of Quebec in Montreal, Montreal, QC;* ²*Hospital Research Center of the University of Montreal, Ophthalmology department, Montreal, QC;* ³*CERMO-FC, Centre d'Excellence de Recherche sur les Maladies Orphelines-Fondation Courtois, Montreal, QC*
- MP 043 **Direct Determination of 4-Beta-Hydroxycholesterol without Derivatization in Human Plasma by LC-APCI-MS/MS;** Jingguo Hou¹; Zhu Xiaodong¹; Bian Alicia¹; Perry Fan¹; Andrew Cunningham¹; ¹*Worldwide Clinical Trials, Austin, TX*
- MP 044 **Exploring protein expression across multiple experiments using Mass Dynamics;** Anna Quagliari¹; Aaron Triantafyllidis¹; Bradley Green¹; Mark Rocco Condina¹; Paula Burton Ngov¹; Giuseppe Infusini¹; Andrew Ian Webb^{1,2,3}; ¹*Mass Dynamics, Melbourne, Australia;* ²*Walter and Eliza Hall Institute, Melbourne, Australia;* ³*Department of Medical Biology, University of Melbourne, Melbourne, Australia*
- MP 045 **Minimum Required Dilution, Matrix Effect and Parallelism Evaluation in Regulated LC-MS Assay for Endogenous Biomarker;** Moucun Yuan¹; Kumar Shah¹; Guoyan Xu¹; William R. Mylott Jr. ¹; ¹*PPD, part of Thermo Fisher Scientific, Richmond, VA*
- MP 046 **Novel LC-MS-PRM method for simultaneous protein quantification using a synaptic and lysosomal panel assay;** Johanna Nilsson¹; Johan Gobom¹; Gunnar Brinkmalm¹; Henrik Zetterberg^{1,2,3,4}; Kaj Blennow¹; Ann Brinkmalm¹; ¹*Institute of Neuroscience and Physiology, Department of Psychiatry and Neurochemistry, University of Gothenburg, Mölndal, Sweden;* ²*UK Dementia Research Institute at University College London, London, United Kingdom;* ³*Department of Neurodegenerative Disease, UCL Institute of Neurology, London, United Kingdom;* ⁴*Hong Kong Center for Neurodegenerative Diseases, Hong Kong, China*
- MP 047 **Quantitative Targeted Proteomics of Mouse Plasma Protein Biomarkers by using Nano LC coupled to Triple Quadrupole Mass Spectrometer;** Xi Qiu¹; Thomas Walker²; Claudia Gaither^{3,4}; Robert Popp³; Christoph H. Borchers⁵; John Sausen⁶; ¹*Agilent Technologies, Wilmington, DE;* ²*Agilent Technologies, Lexington, MA;* ³*MRM Proteomics Inc., Montréal, QC;* ⁴*University of Montreal, Montreal, QC;* ⁵*McGill University, Montreal, Québec;* ⁶*Agilent Technologies, Inc, Santa Clara, California*
- MP 048 **Reduced Ion Suppression in an Automated Extraction of Vitamins B1 and B6 from Whole Blood for LCMS Analysis;** Kyle Dukes; *Biotage, Charlotte, NC*
- MP 049 **Analysis of Frataxin Proteoforms in Human Heart with Pig Heart Surrogate Matrix to Monitor Gene Therapy of Friedreich's Ataxia;** Teerapat Rojsajakul¹; Clementina Mesaros¹; Ian Alexander Blair¹; ¹*University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*
- MP 050 **Comparison of Some Derivatives for the Quantitative Analysis of Short-Chain Fatty Acids (SCFA) by LC/MS/MS;** Anna M. Caldwell¹; John M. Halket¹; Ana Rodriguez-Mateos¹; ¹*King's College London, London, United Kingdom*
- MP 051 **Development of a Comprehensive Quantification Assay for Fast Plasma Protein Screening Using a Novel Triple Quadrupole LC/MS;** Linfeng Wu¹; Guannan Li¹; Patrick Batoon¹; ¹*Agilent Technologies, Santa Clara, CA*
- MP 052 **Development of a Quantitative Biomarker Assay for Marmoset Metabolism;** Robin Goy^{1,2}; Amita Kapoor^{1,2}; ¹*University of Wisconsin-Madison, Madison, WI;* ²*Wisconsin National Primate Research Center, Madison, WISCONSIN*
- MP 053 **Extensive thiol profiling for assessment of intracellular redox status in cultured cells by HPLC-MS/MS;** Jiandong Wu¹; Anna Chernatynskaya¹; Annalise Pfaff¹; Huarui Kou¹; Nan Cen¹; Nuran Ercal¹; Honglan Shi¹; Hu Yang¹; ¹*Missouri University of Science and Technology, Rolla, MO*
- MP 054 **Fast determination of plasma catecholamines and metanephrines by solid-phase extraction and liquid chromatography-tandem mass spectrometry applied to clinical assay;** Thibaut Duval¹; Aziz Kinani²; Laura Akbal¹; Guillaume Chaplain²; Olivier Deschamps³; ¹*Shimadzu France, Noisiel, France;* ²*Cerba, Saint-Ouen-l'Aumône, France;* ³*Biotage, Uppsala, Sweden*
- MP 055 **Investigation of deep proteomic and peptidomic signatures of urine specimen from chronic kidney disease and bladder cancer for disease prediction;** Roland Bruderer¹; Dominic Hoch²; Luca Raess¹; Marco Tognetti¹; Claudia Moresi¹; Yuehan Feng¹; Lukas Reiter¹; ¹*Biognosys AG, Schlieren, Switzerland;* ²*Thermo Fisher Scientific, Reinach, Switzerland*
- MP 056 **Mass spectrometry approaches for the quantification of Neurofilament-light in cerebrospinal fluid: towards a reference method;** Salomé Coppens¹; Jerome Vialaret²; Sylvain Lehmann²; Christophe Hirtz²; Christopher Hopley¹;

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- MP 057 ¹National Measurement Laboratory, LGC, Teddington, United Kingdom; ²Plateforme de Protéomique Clinique (PPC) Univ Montpellier, CHU Montpellier, INM INSERM, Hôpital St Eloi, IRMB, Montpellier, France
Nanoparticles as alternative affinity reagents for developing targeted mass spectrometric assays of low-abundance biomarkers; Shane S Kelly¹; Tai-Tu Lin¹; Matthew J Gaffrey¹; Wei-Jun Qian¹; ¹Pacific Northwest National Laboratory, Richland, WA
- MP 058 **promor: An R package for label-free proteomics data analysis and building machine learning models with candidate proteins;** Chathurani Ranathunge¹; Sagar S Patel¹; Lubna Pinky^{1,2}; Vanessa L Correll¹; Shimin Chen¹; O. John Semmes¹; Robert K Armstrong¹; C. Donald Combs¹; Julius O Nyalwidhe¹; ¹Eastern Virginia Medical School, Norfolk, VA; ²Meharry Medical College, Nashville, TN
- MP 059 **Quantitation of Gal-1P by LC-MS/MS to evaluate GALT activity after AAV Treatment;** Allison N Schorzman¹; Jennifer Franks¹; Jeremy Rouse¹; Kirsten Romero²; Eric Yearley¹; David Scott¹; Michael Guerrero¹; Clayton Beard¹; ¹BridgeBio Gene Therapy, Raleigh, NC; ²BeiGene, Cambridge, MA
- MP 060 **The Urinary Post-translational Modification Landscape and Applications in Clear Cell Renal Cell Carcinoma Biomarker Discovery;** Daniel J Geiszler¹; Nazlı Ezgi Özkan-Küçük¹; Gamze Nur Yapici¹; Murat Can Kiremit¹; Nurhan Ozlu¹; ¹Koc University, Sariyer, Turkey
- MP 061 **Utilizing structural mass spectrometry to probe the dynamics of the progesterone receptor transcription complex;** Matthew D Mann^{1,2}; Min Wang³; Anna Malovannaya³; Raj Kumar⁴; Dean P Edwards³; Patrick R Griffin^{1,2}; ¹Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; ²The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL; ³Baylor College of Medicine, Houston, TX; ⁴Touro College of Pharmacy, New York, NY
- MP 062 **Development of whole blood HR-HRPF for structural pharmacology of protein pharmaceuticals;** Darrienne M Martin; University of Mississippi, University, MS
- MP 063 **Conformational dynamics of the activated GLP-1 receptor-Gs complex revealed by cross-linking mass spectrometry and integrative structure modeling;** Shijia Yuan¹; Lisha Xia¹; Chenxi Wang¹; Liping Sun¹; Wenqing Shui¹; ¹ShanghaiTech University, Shanghai, China
- MP 064 **Evaluation of viral and allergenic protein complexes by dual cleavable crosslinking technology (DUCCT);** Akash Talukder¹; Fnu Ashima¹; Adway O. Zacharias¹; Saiful M Chowdhury¹; ¹University of Texas at Arlington, Arlington, TX
- MP 065 **Expanding the protein crosslinking tool kits by developing a tyrosine reactive crosslinker;** Adway O. Zacharias¹; Saiful Chowdhury²; ¹University of Texas at Arlington, Arlington, TX; ²University of Texas at Arlington, Arlington, TX
- MP 066 **Characterization of Protein-Protein Interactions by Quantitative Cross-linking Mass Spectrometry in Alzheimer's Disease;** Zexin Zhu¹; Bin Wang¹; Xiaofang Zhong¹; Lingjun Li^{1,2}; ¹University of Wisconsin-Madison, School of Pharmacy, Madison, WI; ²University of Wisconsin-Madison, Department of Chemistry, Madison, WI
- MP 067 **Structural interactomic profiling of the synapse by cross-linking mass spectrometry;** Ke Wang¹; Cong Wang¹; Ying Zhu¹; Fan Liu¹; ¹Leibniz-Forschungsinstitut für Molekulare Pharmakologie im Forschungsverbund Berlin e.V. (FMP), Berlin, Germany
- MP 068 **Mapping the multiple DNA contacts made by the neuronal regulatory protein MeCP2 using protein oxidative footprinting;** Yan Sun¹; Sergei Khrapunov¹; Subray Hegde¹; Simone Sidoli¹; Michael Brenowitz¹; ¹Albert Einstein College of Medicine, Bronx, NY
- MP 069 **FOX Photolysis System-Generated Carbene Footprinting of Peptides;** Lyle W Tobin¹; Sandeep K. Misra²; Joshua S. Sharp²; ¹University of Mississippi, University; ²University of Mississippi, University, MS
- MP 070 **Structural mass spectrometry justification of AlphaFold generated PsbS structure on the elongated stromal loop region;** Manjula Mummadisetti¹; Yanchun Lin²; Masakazu Iwai^{3,4}; Krishna K Niyogi^{3,4}; Michael L. Gross²; Haijun Liu⁵; ¹Bioagilytix, Raleigh, NC; ²Department of Chemistry, Washington University in St. Louis, St. Louis, MO; ³Department of Plant and Microbiology, University of California, Berkeley, Berkeley, CA; ⁴Molecular Biophysics and Integrated Bioimaging Division, Lawrence Berkeley National Laboratory, Berkeley, CA; ⁵Department of Biology, Washington University in St. Louis, St. Louis, MO
- MP 071 **RNA-protein crosslinking mass spectrometry - quantification of crosslinking sites;** Luisa Mathilde Welp^{1,2}; Aleksandar Chernev¹; Timo Sachsenberg^{3,4}; Monika Raabe¹; Arslan Siraj^{3,4}; Aditi Sharma⁵; Bernard Delanghe⁵; Rosa Viner⁶; Oliver Kohlbacher^{3,4}; Hennig Urlaub^{1,2}; ¹Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; ²Institute for Clinical Chemistry, University Medical Center Göttingen, Göttingen, Germany; ³Applied Bioinformatics, Department for Computer Science, University of Tübingen, Sand 14, 72076, Tübingen, Germany; ⁴Institute of Bioinformatics and Medical Informatics, University of Tübingen, Tübingen, Germany; ⁵Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ⁶ThermoFisher Scientific, San Jose, California
- MP 072 **Exploring an alternative cysteine-reactive chemistry to enable proteome-wide PPI analysis by cross-linking mass spectrometry;** Fenglong Jiao¹; Leah J. Salituro²; Clinton Yu¹; Craig B. Gutierrez¹; Scott D. Rychnovsky²; Lan Huang¹; ¹Department of Physiology and Biophysics, University of California, Irvine, IRVINE, CA; ²Department of Chemistry, University of California, Irvine, Irvine, CA
- MP 073 **Improved Methods for Residue-Level Mass Spectrometry Data Acquisition and High-Resolution Hydroxyl Radical Protein Footprinting (HRPF) Data Interpretation;** Zhi Cheng¹; Emily Chea¹; Jiana Duan¹; Sandeep K. Misra²; Scot Weinberger¹; Joshua S. Sharp^{1,2}; ¹GenNext Technology, Half Moon Bay, CA; ²University of Mississippi, University, MS
- MP 074 **Mass Spectrometric Footprinting of Protein Adsorption and Desorption at Chromatographic Interfaces;** Kimber N. Focke¹; Brian T. Cooper¹; ¹UNC Charlotte, Charlotte, NC
- MP 075 **Mass spectrometry-based footprinting methods characterize the interaction between human cytochrome P450 enzymes and their redox partner cytochrome P450 reductase;** Mengqi Chai¹; Sarah Burris-Hiday²; Emily E. Scott²; Michael L. Gross¹; ¹Washington University in St. Louis, Saint Louis, MO; ²University of Michigan, Ann Arbor, MI
- MP 076 **AZURIN: A MODEL METALLOPROTEIN TO STUDY AN OLIGOMERIZATION PROCESS;** Roman Tuzhilkin¹; Vladimir Ondruska¹; Jiri Hudecek¹; Miroslav Sulc¹; ¹Department of Biochemistry, Charles University, Prague, Czech Republic
- MP 077 **Crosslinking-MS Captures Transient Interactions within Phase Separated Viral Replication Factories;** Nicole D. Wagner¹; Austin B. Moyle^{1,2}; Chao Wu³; Gaya K. Amarasinghe³; Daisy W Leung³; Michael L Gross¹; ¹Washington University in St. Louis, St. Louis, MO; ²AbbVie Inc., North Chicago, IL; ³Washington University School of Medicine, St. Louis, MO
- MP 078 **Kinase phosphoprobng for profiling protein conformational changes;** Asato Maeda¹; Kosuke Ogata¹; Naoyuki Sugiyama¹; Yasushi Ishihama^{1,2}; ¹Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; ²National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan
- MP 079 **Characterization of Varroa destructor proteins targeted by new acaricides.;** Osei Boakye Fordwour¹; Leonard

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- MP 080 Foster¹; Erika Plettner²; ¹UBC, Vancouver; ²Simon Fraser University, Burnaby, BC
Towards a global phosphoproteomic map of chemotherapy-specific signaling responses; William Comstock¹; Ethan J Sanford¹; Yiseo Rho¹; Marcus Bustamante Smolka¹; ¹Cornell University, Ithaca, NY
- MP 081 **Comprehensive proteome analysis of few neutrophils exposed to melanoma cells of various aggressiveness; Susmita Ghosh¹; Zülal Cibir²; Laxmikanth Kollipara³; Matthias Gunzer^{1,2}; Albert Sickmann¹; ¹Leibniz Institute for Analytical Sciences - ISAS, Dortmund, Germany; ²University of Duisburg-Essen, Essen, Germany; ³Leibniz Institute for Analytical Sciences - ISAS, Dortmund, Germany**
- MP 082 **Identification of Putative Early-Stage Ovarian Cancer Biomarkers Using Bottom-Up Proteomics from Patient Derived Tampons; Gordon T Luu¹; Chang Ge²; Yisha Tang²; Andrew K Godwin^{3,4}; Judith Su⁵; Laura M Sanchez¹; ¹University of California Santa Cruz, Santa Cruz, CA; ²University of Arizona, Tucson, AZ; ³University of Kansas Medical Center, Kansas City, KS; ⁴University of Kansas Cancer Center, Kansas City, KS; ⁵University of Arizona, Tucson, AZ**
- MP 083 **Photobleaching and photoproducts analyses of the photosensitizers, protoporphyrin IX and protoporphyrin IX dimethyl ester, for photodynamic diagnosis/therapy of cancers; Sochi J Ogbonna¹; Hisanao Hazama¹; Katsuyoshi Masuda^{1,2}; Kunio Awazu^{1,3}; ¹Graduate School of Engineering, Osaka University, Suita, Japan; ²Graduate School of Medicine, Kyoto University, Kyoto, Japan; ³Global Center for Medical Engineering and Informatics, Osaka University, Suita, Japan**
- MP 084 **Quantitative analysis of extracellular matrix-enriched fresh tissues and formalin-fixed paraffin-embedded tissues reveals distinct protein signatures of lung cancers; Samah Shah¹; Deng Pan²; Joanna Bons¹; Jacob P. Rose¹; Rosemary Bai²; Chira Chen-Tanyolac²; Xianhong Wang²; Veena Sangwan³; Sophie Camilleri-Broët⁴; Philippe Gascard²; Lorenzo Ferri³; Thea D Tlsty²; Birgit Schilling¹; ¹Buck Institute for Research on Aging, Novato, CA; ²Department of Pathology, University of California, San Francisco, CA; ³Division of Thoracic and Upper Gastrointestinal Surgery, Montreal General Hospital, McGill University Health Centre, Montreal, QC; ⁴Department of Pathology, McGill University, Montreal, QC**
- MP 085 **Establishing proteome divergence between high-grade serous ovarian tumors and their patient-derived xenograft experimental models; Jesenia M Perez¹; Joohyun Ryu²; Mihir Shetty^{3,4}; Boris Winterhoff^{3,4}; Timothy K. Starr^{3,4}; Stefani N. Thomas²; ¹Microbiology, Immunology, and Cancer Biology Program, University of Minnesota, Minneapolis, MN; ²Department of Laboratory Medicine and Pathology, University of Minnesota, Minneapolis, MN; ³Department of Obstetrics, Gynecology and Women's Health University of Minnesota, Minneapolis, MN; ⁴Masonic Cancer Center, University of Minnesota, Minneapolis, MN**
- MP 086 **Quantification of Cross-Tissue Extracellular Matrix Alterations Associated with Malignancy in Human Chronic Inflammation-Associated Cancers using an Optimized Data-Independent Acquisition Workflow; Joanna Bons¹; Deng Pan²; Samah Shah¹; Rosemary Bai²; Chira Chen-Tanyolac²; Nathan Basisty¹; Amy O'Broin¹; Jacob P. Rose¹; Veena Sangwan³; Sophie Camilleri-Broët⁴; Philippe Gascard²; Lorenzo Ferri³; Thea D. Tlsty²; Birgit Schilling¹; ¹Buck Institute for Research on Aging, Novato, CA; ²Department of Pathology, University of California, San Francisco, CA; ³Division of Thoracic and Upper Gastrointestinal Surgery, Montreal General Hospital, McGill University Health Centre, Montreal, QC; ⁴Department of Pathology, McGill University, Montreal, QC**
- MP 087 **Intra- and Inter-Patient Tumor Proteome Heterogeneity in Metastatic Lung Cancer; Sudhir Putty Reddy¹; Hilal Ozakinci¹; Lamees Saeed¹; Bin Fang¹; Victoria Izumi¹; Joseph Johnson¹; Brooke Smedley¹; Eric Welsh¹; Steven Eschrich¹; Eric Haura¹; Theresa Boyle¹; John M Koomen¹; ¹H. Lee Moffitt Cancer Center, Tampa, FL**
- MP 088 **Surfaceome Enrichment Strategies for Discovery of Immunotherapy Targets in Multiple Myeloma; Bin Fang¹; Eric Welsh¹; Umasangtongkul Sura-Attha¹; Mark Meads¹; Meghan Menges¹; Alugubelli Raghunandan Reddy¹; Frederick Locke¹; Ken Shain¹; John M Koomen¹; Ciara L Freeman¹; ¹H. Lee Moffitt Cancer Center, Tampa, FL**
- MP 089 **Spatially resolved multi-omic imaging of glioblastoma multiforme to examine hypoxic signatures; Caroline Pollard¹; Rory T Steven²; Alina Finch³; Laura Porto³; Victoria Wykes³; Colin Watts³; Sabrina Nayer⁴; Joe Flint⁴; Jack McMurray⁴; Andrew Filer⁴; Daniel A Tennant⁵; Josephine Bunch²; ¹National Physical Laboratory, Teddington, United Kingdom; ²National Physical Laboratory, Teddington, United Kingdom; ³Institute of Cancer and Genomic Science, University of Birmingham, Birmingham, United Kingdom; ⁴Institute of Inflammation and Ageing, University of Birmingham, Birmingham, United Kingdom; ⁵Institute of Metabolism and Systems Research, University of Birmingham, Birmingham, United Kingdom**
- MP 090 **PSA proteomics between cancer tissues and blood among 20 prostate cancer patients for early diagnosis; Wonryeon Cho¹; Miseon Jeong¹; WONKWANG UNIVERSITY, Iksan, South Korea**
- MP 091 **Comparative Analysis of Tumours, Their Metastases and Derived Primary Cell Lines by Rapid Evaporative and Desorption Electrospray Ionization Mass Spectrometry; Adrienn Molnár^{1,2}; Gabriel Stefan Horkovics-Kovats^{1,2}; Nóra Kucsma³; Richard Schäffer¹; Zsuzsanna Szegő¹; Attila Egri¹; Gitta Schlosser²; Gergely Szakács^{3,4}; Bálint András Deák⁵; Júlia Balog¹; ¹Waters Research Center, Budapest, Hungary; ²ELTE Eötvös Loránd University, Budapest, Hungary; ³ELKH Research Centre for Natural Sciences, Institute of Enzymology, Budapest, Hungary; ⁴Center for Cancer Research, Medical University of Vienna, Vienna, Austria; ⁵Department of Pathology, Forensic and Insurance Medicine, Semmelweis University, Budapest, Hungary**
- MP 092 **Advancing precision medicine in colorectal cancer using ambient ionisation mass spectrometry and high-throughput personalised in vitro metabolomics; Stefania Maneta-Stavarakaki¹; Annalisa Lorenzato²; Daniel Simon¹; Yuchen Xiang¹; Mariangela Russo²; Andrew Campbell³; Owen Sansom³; Alberto Bardelli²; Zoltan Takats¹; ¹Imperial College London, London, United Kingdom; ²University of Turin, Turin, Italy; ³Beaton Institute for Cancer Research, Glasgow, United Kingdom**
- MP 093 **Proteomic Signatures for Diagnosing and Monitoring Treatment of Human Bladder Cancer; Onika Noel¹; Susan T. Weintraub¹; Harshit Garg¹; Furkan Dursun¹; Dharam Kaushik¹; Sammy Pardo¹; Dana Molleur¹; Michael Liss¹; Robert Svatek¹; Ahmed Masour¹; ¹Univ. of Texas HSC, San Antonio, TX**
- MP 094 **TMT Proteomics and Phosphoproteomics identifies LIN28A and STAT3 synergistically confer Chronic Myeloid Leukemia Resistance; Owen J.H. Hovey¹; Mallory I Frederick²; Jenica H Kakadia²; Tingting Wu¹; Courtney Voss¹; Ilka U Heinemann¹; Shawn S.C. Li¹; ¹University of Western Ontario, London, ON; ²University of Western Ontario, London, ON**
- MP 095 **Prolyl Isomerase Pin1 is involved in regulating PML-NB dynamics during senescence; Rodrigo Mohallem¹; Uma K Aryal¹; ¹Purdue University, West Lafayette, Indiana**
- MP 096 **Extensive Three-Dimensional Intratumor Proteomic Heterogeneity Revealed by Multiregion Sampling in Uterine Serous Tumor Specimens; Allison L Hunt^{1,2}; Nicholas W. Bateman^{2,3,4}; Waleed Barakat^{3,4,5}; Sasha C. Makohon-Moore^{2,3,4}; Tamara Abulez^{2,3,4}; Brian L. Hood^{2,3,4}; Kelly A. Conrads^{2,3,4}; Ming Zhou^{1,2}; Jeremy Loffredo^{2,3,4}; Katlin N. Wilson^{2,3,4}; Tracy J. Litz^{2,3,4}; Neil T. Phippen²; Emanuel F. Petricoin⁶; Uma N.M. Rao^{2,3}; G. Larry Maxwell¹**

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- ^{2,4}; Thomas P. Conrads^{1,2,4}; ¹Women's Health Integrated Research Center, Inova Women's Service Line, Inova Health System, Annandale, Virginia; ²Women's Health Integrated Research Center, Gynecologic Cancer Center of Excellence, Department of Obstetrics and Gynecology, Uniformed Services University and Walter Reed National Military Medical Center, Bethesda, Maryland; ³The Henry M. Jackson Foundation for the Advancement of Military Medicine, Inc., Bethesda, Maryland; ⁴The John P. Murtha Cancer Center Research Program, Department of Surgery, Uniformed Services University, Bethesda, Maryland; ⁵Women's Health Integrated Research Center, Gynecologic Cancer Center of Excellence, Department of Obstetrics and Gynecology, Uniformed Services University and Walter Reed National Military Medical Center, Annandale, Virginia; ⁶Center for Applied Proteomics and Molecular Medicine, George Mason University, Manassas, Virginia
- MP 097 **Using substrate trapping to identify HDAC6 interactors in the setting of BRCA-1/2 wildtype high-grade serous ovarian cancer;** Jolene M Duda¹; Stefani N. Thomas¹; ¹University of Minnesota, Minneapolis, MN
- MP 098 **Mass spectrometry imaging combined with orthogonal techniques identifies therapeutic vulnerabilities in the pediatric brain tumor, embryonal tumor with multilayered rosettes;** Kelly C O'Neill¹; Evangelos Liapis¹; Annapurna Pamreddy¹; Allison Maas¹; Derek Hanson¹; Claire Louise Carter¹; ¹Hackensack Meridian Center for Discovery & Innovation, Nutley, NJ
- MP 099 **Proteomic Characterization of the Tumor Microenvironment in Patients with Oral Squamous Cell Carcinoma;** Allison L Hunt^{1,2}; Tamara Abulez^{1,3,4}; Kelly A. Conrads^{1,3,4}; Katlin N. Wilson^{1,3,4}; Brian L. Hood^{1,3,4}; Nicholas W. Bateman^{1,3,4}; Jaeil Ahn⁵; Julius Benicky^{6,7}; Thomas P. Conrads^{1,2,4}; Radoslav Goldman^{6,7,8}; ¹Women's Health Integrated Research Center, Gynecologic Cancer Center of Excellence, Department of Obstetrics and Gynecology, Uniformed Services University and Walter Reed National Military Medical Center, Bethesda, Maryland; ²Women's Health Integrated Research Center, Inova Women's Service Line, Inova Health System, Annandale, Virginia; ³The Henry M. Jackson Foundation for the Advancement of Military Medicine, Inc., Bethesda, Maryland; ⁴The John P. Murtha Cancer Center Research Program, Department of Surgery, Uniformed Services University, Bethesda, Maryland; ⁵Department of Biostatistics, Bioinformatics and Biomathematics, Georgetown University, Washington, DC; ⁶Department of Oncology, Lombardi Comprehensive Cancer Center, Georgetown University, Washington, DC; ⁷Clinical and Translational Glycoscience Research Center, Georgetown University, Washington, DC; ⁸Department of Biochemistry and Molecular & Cell Biology, Washington, DC
- MP 100 **Metabolomic profiling of patient-matched primary and recurrent glioblastoma reveals dynamic metabolic reprogramming through therapy;** Olivia Taverniti¹; William D. Gwynne¹; Andrew T. Quail¹; William T. Maich²; Zsolt Zador²; Sheila K. Singh²; J. Rafael Montenegro-Burke¹; ¹Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; ²Center for Discovery in Cancer Research, McMaster University, Hamilton, ON
- MP 101 **Investigating the Role of Proteins in Regulating Breast Density in Premenopausal Breast Cancer Patients;** Minsoo Son¹; Antonia Zamacona Calderon¹; Adetunji Toriola²; Young Ah Goo¹; ¹MTAC, MGI, Washington University School of Medicine in Saint Louis, Saint Louis, MO; ²Washington University School of Medicine, St. Louis, MO
- MP 102 **Alterations in glutamate to glutamine ratios detected by DESI and MSPen allow diagnosis and molecular subtyping of breast cancer;** Keziah E Liebenberg¹; Erin Craig²; Meredith L Spradlin¹; Michael F Keating¹; Robert Tibshirani²; Livia S. Eberlin¹; ¹Baylor College of Medicine, Houston, TX; ²Stanford University, Stanford, CA
- MP 103 **Therapeutic targeting of lipid saturation in recurrent MYC-amplified medulloblastoma;** William D. Gwynne¹; Jeremy K Chan¹; Stefan Custers²; Andrew T Quail¹; Chitra Venugopal²; Sheila K. Singh²; J. Rafael Montenegro-Burke¹; ¹Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; ²Center for Discovery in Cancer Research, McMaster University, Hamilton, ON
- MP 104 **Enhanced glucose oxidation in Birt-Hogg-Dubé syndrome renal tumors revealed by Ion-Chromatography coupled with Ultra-High-Resolution Mass Spectrometry based Stable-Isotope-Resolved Metabolomics;** Ye Yang¹; Daniel R. Crooks¹; Laura S. Schmidt^{1,2}; Richard M. Higashi³; Teresa W-M. Fan³; Andrew N. Lane³; Youfeng Yang¹; Cathy D. Vocke¹; W. Marston Linehan¹; ¹Urologic Oncology Branch, Center for Cancer Research, National Cancer Institute, National Institutes of Health, Bethesda, Maryland; ²Basic Science Program, Frederick National Laboratory for Cancer Research, Frederick, Maryland; ³Department of Toxicology and Cancer Biology, Markey Cancer Center, University of Kentucky, Lexington, Kentucky
- MP 105 **Molecular correlates for head and neck squamous cell carcinoma engraftment are associated with patient outcomes;** Matthew Waas¹; Christina Karamboulas²; Laurie Ailles^{2,3}; Thomas Kislinger^{1,2}; ¹Princess Margaret Cancer Centre, Toronto, ON; ²University of Toronto, Toronto, ON; ³Princess Margaret Cancer Centre, University Health Network, Toronto, ON
- MP 106 **Characterization of Metabolic Heterogeneity in Pediatric Hepatoblastoma;** Trevor M. Godfrey¹; Andres F. Espinoza^{1,2}; Sarah E. Woodfield^{1,2}; Sanjeev A. Vasudevan^{1,2}; Livia S. Eberlin¹; ¹Baylor College of Medicine, Houston, TX; ²Texas Children's Hospital, Houston, TX
- MP 107 **Preoperative Classification of Thyroid Nodules by DESI-MS Imaging of Fine Needle Aspiration Biopsies;** Rachel J. Dehoog¹; Ahmed Al-Fartosi¹; Neda Zarrin-Khameh¹; Rongrong Huang¹; Livia S. Eberlin¹; James Suliburk¹; ¹Baylor College of Medicine, Houston, TX
- MP 108 **Application of Magnetic Beads in Automated Sample Preparation for Simultaneous Extraction of Angiotensin I and Steroids in Plasma by LC-MS/MS;** Pengyun Liu¹; Xiaofen Yuan¹; Weijia Wu¹; Huaifen Liu¹; ¹Calibra Diagnostics, Hangzhou, China
- MP 109 **Classifying membranous nephropathy by mass spectrometry;** Aaron J Storey¹; Samar Hassen²; Christian Herzog¹; John M Arthur¹; Rick D Edmondson¹; Tiffany N Caza²; Chris P Larsen²; ¹University of Arkansas for Medical Sciences, Little Rock, AR; ²Arkana Laboratories, Little Rock, AR
- MP 110 **Mass Spectrometry Imaging Guided Spatial Proteomics for Stratification of Patient with Glioblastoma and Identification of Prognosis Markers;** Marie Duhamel¹; Maxence Wisztorski¹; Isabelle Fournier¹; Michel Salzet¹; ¹PRISM Inserm U1192 - University of Lille, Villeneuve D'ascq Cedex, France
- MP 111 **Gas Chromatography Rapid Automation and Quantitative Procedure for the Measurement of Hydrogen Cyanide in Whole Blood;** Paul Brito-Vargas¹; James Lapalme¹; Elizabeth Bair¹; Ona Adair¹; Nicolas Epie¹; ¹South Carolina Public Health Laboratory, Columbia, SC
- MP 112 **Finger-Sticking Good: Clinical Fatty Acids GC-MS Analysis from a Dried Microsample;** Meghan Bradley¹; Matthew L. Crawford¹; Christopher M. Shuford¹; Russell P. Grant¹; ¹LabCorp, Burlington, NC
- MP 113 **Adapting the MasSpec Pen for Non-destructive Screening of Oral Premalignancies (OPMDs) to Identify Oral Cavity Squamous Cell Cancers (OSCC);** Charles A. Wolfe¹; Michael F. Keating²; Gabrielle Wolter³; Erich M. Sturgis³; Carlos Chone⁴; Livia S. Eberlin¹; ¹Department of Surgery, Baylor College of Medicine, Houston, TX;

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- ²University of Texas at Austin, Austin, TX; ³Department of Otolaryngology, Baylor College of Medicine, Houston, Texas; ⁴Department of Otolaryngology, University of Campinas, Campinas, Brazil
- MP 114 **Multiplexed targeted assay for detection of sphingolipids**; Seul Kee Byeon¹; Kimiyo Raymond¹; Devin Oglesbee¹; Matthew Schultz¹; Dietrich Matern¹; Akhilesh Pandey¹; ¹Mayo Clinic, Rochester, MN
- MP 115 **Microprobe-Capture In-Emitter Elution Coupled with Mass Spectrometry for Structural Elucidation and Clinical Testing of β 2-Transferrin**; Ruben Y Luo^{1,2}; Christopher Pfaffroth²; Samuel Yang¹; Kevin Hoang²; Priscilla SW Yeung^{1,2}; James Zehnder^{1,2}; Run-Zhang Shi^{1,2}; ¹Stanford University, Palo Alto, CA; ²Stanford Health Care, Palo Alto, CA
- MP 116 **Development of 3D Microfluidic Paper-based Analytical devices (μ PADs) with Mass Spectrometric Signal Amplification for diagnosis of Malaria in clinical setting**; Avesha Seth¹; Abraham Kwame Badu-Tawiah¹; ¹The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH
- MP 117 **Determination of 18 Steroid Hormones in Human Serum Using Rapid Protein Precipitation Method in Coupled With Liquid Chromatography-Tandem Mass Spectrometry**; Dan Liu¹; Fengmei Hu²; Chao Huang²; Xianglong Zhao²; ¹Shanghai AB SCIEX, Shanghai, China; ²China AB SCIEX, Shanghai, China
- MP 118 **Therapeutic Drug Monitoring (TDM) of 26 medications in urine samples of hypertensive patients using LC-MS/MS for medication adherence**; Yi Ting Tan¹; Troy Puar¹; Daryl Hee¹; ¹Changi General Hospital, Singapore, Singapore
- MP 119 **Acylcarnitines in Dried Blood Spots (DBS) Samples by FIA-MS/MS: Convenient use of Single Stable Isotope Labeled Internal Standards CRM Mix**; Arun Babu Kumar¹; Lauren Lytwak¹; Sarah Aijaz¹; Uma Sreenivasan¹; ¹MilliporeSigma, Round Rock, TX
- MP 120 **Rapid Diagnosis of Cytologically Indeterminate Thyroid Fine-Needle Aspiration Biopsies using Paper Spray Ionization Miniature Mass Spectrometry**; Jia-Ying Yu¹; Laura Min Xuan Chai¹; Ming-Hsun Wu²; Kuen-Yuan Chen²; Cheng-Chih Hsu¹; ¹National Taiwan University, Taipei, Taiwan; ²National Taiwan University Hospital, Taipei, Taiwan
- MP 121 **Generic Methods for Simultaneous Analysis of Four Direct Oral Anticoagulants in Human Plasma and Urine by UPLC-Tandem Mass Spectrometry**; Xin Zheng¹; Xinge Cui¹; ¹Peking Union Medical College Hospital, Beijing, China
- MP 122 **Quantification of therapeutic proteins with a focus on TDM**; Albert Sickmann¹; Rob Dahlmann^{2,3}; Phil Carbow^{3,4}; Roman Sakson^{4,5}; Yvonne Reinders⁴; ¹Leibniz-Institut für Analytische Wissenschaften -, Dortmund, Germany; ²Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund 44139, Germany, Dortmund, Germany; ³University of Applied Science, Hamm-Lippstadt, Hamm, Germany; ⁴ISAS- Leibniz Institut für Analytische Wissenschaften, Dortmund, Germany; ⁵University of Applied Science, Mannheim, Germany
- MP 123 **Predicting Septic Shock in Emergency Patients with Serum Metabolic Profiles and Machine Learning**; Yu Hong¹; Li-Hua Li²; Ting-Hao Kuo¹; Yi-Tzu Lee^{3,4}; Cheng-Chih Hsu¹; ¹Department of chemistry, National Taiwan University, Taipei, Taiwan; ²Department of Pathology and Laboratory Medicine, Taipei Veterans General Hospital, Taipei, Taiwan; ³Department of Emergency Medicine, Taipei Veterans General Hospital, Taipei, Taiwan; ⁴Faculty of Medicine, School of Medicine, National Yang-Ming University, Taipei, Taiwan
- MP 124 **Simultaneous Quantitation of Renin Activity, Aldosterone and Angiotensin II in Human Plasma Using Rapid Prot**; Fengmei Hu¹; Dan Liu²; Chao Huang²; Xianglong Zhao²; ¹Shanghai AB Sciex Analytical Instrument Trading Co.,Ltd., Shanghai, China, Shanghai, China; ²Shanghai AB Sciex Analytical Instrument Trading Co.,Ltd., Shanghai, China
- MP 125 **Efficient Extraction of Proteins from Desiccated Blood followed by On-Bead Trypsinization - An Efficient Alternative to Plasma-based LC-MS Analysis**; Debadeeep Bhattacharyya¹; Patrick McCarthy¹; Heidi Giese¹; Martina Werner¹; Eugenio Daviso¹; Sameer Vasantgadkar¹; Ulrich Thomann¹; ¹Covaris, Lexington, MA
- MP 126 **Advancing Clinical (Auto)antibody Analysis: Fc-Proteoform Profiling of IgG Allotypes in Rheumatoid Arthritis**; Constantin Blöchl¹; Christoph Gstöttner¹; Eva Maria Stork²; Rayman T. N. Tjokrodirdjo¹; Peter A. van veelen¹; Hans Ulrich Scherer²; Rene E. M. Toes²; Manfred Wuhrer¹; Elena Domínguez-Vega¹; ¹Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; ²Department of Rheumatology, Leiden University Medical Center, Leiden, Netherlands
- MP 127 **Development of direct mass spectrometry platform for shotgun metabolomics analyses of whole blood samples for malaria diagnosis**; Riley Ferguson¹; Abraham Kwame Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- MP 128 **A quantitative detection method for 9 water-soluble vitamins in human serum/plasma**; Cong Xu; *agilent*, Beijing, China
- MP 129 **A semi-automated workflow for targeted LC/MS analysis of circulating bile acids in plasma samples**; Pietro Morlacchi¹; Cate Simmermaker²; Patrick Battoon²; ¹Agilent, Lexington, MA; ²Agilent Technologies, Santa Clara, CA
- MP 130 **Clinical applications utilizing in-pipet dispersive SPE prior to LC-MS/MS**; Yong Chen¹; Hugh Cramer²; M James Ross¹; Gabriel Odugbesi²; ¹MilliporeSigma, Bellefonte, PA; ²Millipore Sigma, Bellefonte, PA
- MP 131 **Determination of nine neurotransmitters in plasma by HPLC ESI-MS/MS**; Ruichen Liu¹; Xuzhe Pei¹; Chao Huang¹; Xianglong Zhao¹; Lihai Guo¹; ¹SCIEX, Beijing, China
- MP 132 **High-throughput profiling of reactive cysteines and lysines by automated proteomics workflow**; Zixiang Fang¹; Taylor P Ma¹; Hanna G Budayeva¹; ¹Genentech, Inc., South San Francisco, CA
- MP 133 **Fast and Sensitive Analysis of FPOP data using MSFragger and FragPipe**; Carolina Rojas Ramirez¹; Daniel A. Polasky²; Jessica Arlett Espino³; Lisa Jones⁴; Alexey I. Nesvizhskii¹; ¹University of Michigan-Ann Arbor, Ann Arbor, MI; ²University of Michigan Ann-Arbor, Ann Arbor, MI; ³University of Maryland, School of Pharmacy, Baltimore, MD; ⁴University of California San Diego, San Diego, CA
- MP 134 **Comparing Common Biophysical Methods to Evaluate MS-based Footprinting-Induced Perturbation of Protein High Order Structure (HOS)**; Wesley J. Wagner¹; Austin B. Moyle^{1,2}; Nicole D. Wagner¹; Michael L. Gross¹; ¹Washington University in St. Louis, St. Louis, MO; ²AbbVie Inc., North Chicago, IL
- MP 135 **Single Sequence Identification of Probe-Modified Peptides by TrypN C-terminal Clipping of Tryptic Peptides**; Clodette Punzalan¹; Mariel Clores¹; Connor Jewell¹; Xudong Yao¹; ¹University of Connecticut, Storrs, CT
- MP 136 **Building fully controlled interactomes and tools to advance protein interaction identification by cross-linking mass spectrometry**; Milan Avila Clasen¹; Max Ruwolt²; Louise Ulrich Kurt¹; Fabio Cesar Gozzo³; Paulo Costa Carvalho¹; Diogo Borges Lima²; Fan Liu²; ¹Laboratory for Structural and Computational Proteomics, Carlos Chagas Institute, Fiocruz, Curitiba, Brazil; ²Department of Structural Biology, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; ³Dalton Mass Spectrometry Laboratory, University of Campinas, Campinas, Brazil

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- MP 137 **Developing LC-MS workflows for cross-link identification from low sample amounts;** Abigail H Lewis¹; Siang-Wun Siao¹; Tomas Koudeka²; Julia Kraegenbring³; Rosa Viner⁴; Ilaria Piazza²; Fan Liu¹; ¹Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany; ²Max Delbrück Center for Molecular Medicine in the Helmholtz Association, Berlin Institute for Medical Systems Biology, Berlin, Germany; ³Thermo Fisher Scientific, Bremen, Germany; ⁴ThermoFisher Scientific, San Jose, CA
- MP 138 **New insight into SARS-CoV-2 interactions with host cells using in vivo Crosslinking Mass Spectrometry;** Martial Rey¹; Florence GUIVEL-BENHASSINE²; Karen Druart¹; Olivier Schwartz²; Julia Chamot-Rooke¹; ¹Mass Spectrometry for Biology Unit, Université Paris Cité, Institut Pasteur, CNRS, UAR 2024, Paris, France; ²Virus and Immunity Unit, Institut Pasteur, Université Paris Cité, CNRS UMR3569, Paris, France
- MP 139 **Comparison of Protein Footprinting Approaches for Epitope Mapping of TNF α /Infliximab complex;** Samantha J Knott¹; Daniel Benjamin¹; Richard Y-C Huang^{2,3}; James Dowell¹; Ekaterina G. Deyanova²; Tahmid Hassan²; Robert Langshir²; Yun Wang²; Faraz Choudhury¹; ¹Immuto Scientific Inc., Madison, WI; ²Bristol Myers Squibb, Princeton, NJ; ³Janssen Pharmaceuticals, Spring House, PA
- MP 140 **Probing Antibody-Host Proteome Interactions via Intracellular Cross-linking;** Bradley Hart¹; Yi He¹; Lauren M Kraft²; Michael Poltash²; Chris Sauer²; Elsa Gorre²; Andrew Mahan²; Thomas Kelly²; Hirsh Nanda²; Rosa Viner¹; Harsha Gunawardena²; ¹ThermoFisher Scientific, San Jose, CA; ²JOHNSON AND JOHNSON, Spring House, PA
- MP 141 **Application of FoxWare® Software for Resolving Isomeric Heterogeneity and Retention Time Drift in Oxidized Peptides from Hydroxyl Radical Protein Footprinting;** Jiana Duan¹; Robert Egan¹; Calyx Liu¹; Tyler Fletcher¹; Emily Chea¹; Sandeep K. Misra²; Joshua Sharp^{1,2}; Scot Weinberger¹; ¹GenNext Technology, Half Moon Bay, CA; ²University of Mississippi, University, MS
- MP 142 **Large scale identification of cross-linked peptides from bovine exosomes using a multi-chromatography approach;** Yiran Ma¹; Noor H. Naseeb¹; Adam J Anthony¹; Andrew D. Couse¹; Jonathan C. Trinidad¹; David E. Clemmer¹; ¹Indiana University, Bloomington, IN
- MP 143 **Benchmarking MS2- and MS3-based acquisition strategies for XL-MS using a developmental ProteinProspector/Touchstone pipeline;** Clinton Yu¹; Mike Trnka²; Peter Baker²; Robert Chalkley²; Al Burlingame²; Lan Huang¹; ¹University of California, Irvine, Irvine, CA; ²University of California San Francisco, San Francisco, CA
- MP 144 **An atlas of reactive and functional chromatin-associated cysteines in cancer;** Daniele Canzani¹; Brian McEllin¹; Erin Broderick¹; Tonibelle Gatbonton-Schwager¹; Yang Gao¹; Julia E Robbins¹; Andrea I Gutierrez¹; Carolyn Allen¹; J. Sebastian Paez¹; William E Fondrie¹; Lindsay K Pino¹; Alexander J Federation¹; ¹Talus Bioscience, Seattle, WA
- MP 145 **Mapping of the Interaction Site of a Novel Fungal Lectin to a Peptidoglycan from *Listera innocua*;** Sandeep K. Misra¹; Sushil K. Mishra¹; Nika Janez²; Robert J. Doerksen¹; Jerica Sabotić²; Joshua S. Sharp¹; ¹University of Mississippi, University, MS; ²Jozef Stefan Institute, Jamova cesta 39, Slovenia
- MP 146 **Identifying the culprits of novel proteolytic activity in secreted proteins of *B. subtilis* using N-terminal covalent labeling;** Matthew Davison¹; Charles Dann²; Jonathan C. Trinidad³; James Reilly³; ¹Indiana University, Bloomington, IN; ²Indiana University Bloomington, Bloomington, Indiana; ³Indiana University Bloomington, Bloomington, IN
- MP 147 **Visualization of transient DOT1A-nucleosome interactions in solution by X-ray protein footprinting;** Janna Kiselar¹; Victoria S Frisbie²; Mark R Chance¹; Hideharu Hashimoto²; Erik W Debler²; ¹Case Western Reserve University, Cleveland, OH; ²Thomas Jefferson University, Philadelphia, PA
- MP 148 **Applying Machine Learning Tools to Analyze Crosslinking and TMT Mass Spectrometry Datasets;** Zhihui Wen¹; Ying Zhang¹; Yan Hao¹; Laurence Florens¹; ¹Stowers Institute for Medical Research, Kansas City, MO
- MP 149 **Protein structure and higher order assembly in Vaccinia virus by combination of XLMS with deep learning protein structure prediction methods;** Yeva Mirzakhanyan¹; Andris Jankevics²; Richard A. Scheltema²; Paul D. Gershon¹; ¹UC-Irvine, Irvine, CA; ²Utrecht University, Utrecht, Netherlands
- MP 150 **Enrichable covalent labeling for efficient global, temporal, in situ profiling of protein structural changes in living cells;** Chengzhi Cai¹; Guoting Qin¹; Shara Duong¹; John Mansour¹; Conor Mullens²; ¹University of Houston, Houston, TX; ²Bruker Daltonics, Billerica, MA
- MP 151 **Mass spectrometry analysis of IgA N-glycans for biomarker discovery: Application in a pilot study to discriminate patients with ankylosing spondylitis;** Hui-Ling Chiang¹; Ming-Chi Lu^{1,2}; Ning-Sheng Lai¹; Chien-hsueh Tung¹; Kuang-Yung Huang¹; Bao-Bao Hsu¹; Chih-Chia Yu²; Yi-Ling Ye³; ¹Division of Immunology, Allergy and Rheumatology, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan; ²Department of Medical Research, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan; ³Department of Biotechnology, National Formosa University, Huwei, Taiwan
- MP 152 **Multi-Omic molecular characterisation of pre-invasive breast ductal carcinoma using tumor micro arrays identifies putative biomarkers and readily druggable targets;** Georgia Mitsa^{1,2}; Livia Florianova³; Josiane Lafleur⁴; Adriana Aguilar-Mahecha⁴; Mark Basik⁵; Gerald Batist^{1,4,6,7}; Christoph H Borchers^{1,2,4,8}; ¹Division of Experimental Medicine, McGill University, Montreal, QC; ²Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ³Department of Pathology, Segal Cancer Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁴Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ⁵Department of Oncology and Surgery, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁶Department of Oncology, McGill University, Montreal, QC; ⁷Exactis Innovation, Montreal, QC; ⁸Department of Oncology and Pathology, Segal Cancer Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC
- MP 153 **A comparative investigation of plasma proteome profiling with state-of-the-art mass spectrometry and affinity-based assays;** Ino Karemaker¹; Roland Bruderer¹; Jakob Vowinckel¹; Karel Novy¹; Kristina Beeler¹; Raphael Heilig¹; Sebastian Müller¹; Lukas Reiter¹; Yuehan Feng¹; ¹Biognosys AG, Schlieren, Switzerland
- MP 154 **Development of an MS-based multimarker glycomics test for earlier detection of pancreatic cancer among high risk individuals and treatment monitoring;** Yuri Van Der Burgt¹; Derk C.F. Klatter¹; Iris J.M. Levink²; Bert A. Busing¹; Wilma E. Mesker¹; Djuna L. Cahen³; Gwenny M. Fuhler³; Marco J. Bruno³; Monique E. Van Leerdam¹; Manfred Wuhrer¹; ¹Leiden University Medical Center, Leiden, Netherlands; ²Erasmus Medical Center Rotterdam, Rotterdam, Netherlands; ³Erasmus Medical Center Rotterdam, Rotterdam, Netherlands
- MP 155 **3-Dimensional Primary Human Chondrocyte Pellets and Cellular Alterations during Osteoarthritis and Senescence;** Jacob P. Rose¹; Sandip Patel¹; Joanna Bons¹; Charles A. Schurman¹; Christina D. King¹; Samah

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- Shah¹; Judith Campisi^{1,2}; Tamara Alliston^{3,4}; Birgit Schilling¹; ¹Buck Institute for Research on Aging, Novato, CA; ²Lawrence Berkeley Laboratory, University of California, Berkeley, CA; ³University of California San Francisco, Department of Orthopaedic Surgery, San Francisco, CA; ⁴UC Berkeley/UCSF Graduate Program in Bioengineering, Berkeley, CA
- MP 156 **Explore protein glycosylation as non-invasive biomarker for chronic liver diseases**; Mark M. Kushnir¹; Carmen Dunbar¹; Yanhong Wu²; Yifei Yang²; ¹ARUP Laboratories, Salt Lake City, UT; ²Mayo Clinic, Rochester, MN
- MP 157 **Combined serum proteome profile of Alzheimer's disease**; Jiayi Zhang¹; Huali Shen¹; ¹Fudan University, Shanghai, China
- MP 158 **Pushing the limits of atmospheric pressure MALDI MS histochemistry on high-resolution OrbitrapTM systems for FFPE patient tissue analysis**; Peter D. Verhaert¹; Raf Sciot²; Gilles Frache³; ¹ProteoFormix, Beerse, Belgium; ²Academic Hospital University of Leuven, Leuven, Belgium; ³Luxembourg Institute of Science and Technology, Belvaux, Luxembourg
- MP 159 **Investigation of Bile Acids of in Public Data related to Neurological Disorders**; Jasmine Jungok Zemlin¹; Pieter C Dorrestein¹; Ipsita Mohanty¹; ¹UCSD, La Jolla, CA
- MP 160 **Deep, Unbiased and Quantitative mass spectrometry-based plasma proteome analyses of adaptive response to COVID-19 vaccine**; Ting Huang¹; Alex Rosa Campos²; Ramon Diaz Pena²; Svetlana Maurya²; Khatereh Motamedchaboki¹; Laura R. S. Oliveira³; Camila I. Alves³; Rafael L. Rosa³; Yohana P. C. Alves³; Lucélia Santi³; Walter O. Beys-da-Silva³; ¹Seer, Inc., Redwood City, CA; ²Sanford Burnham Prebys, San Diego, California; ³Federal University of Rio Grande do Sul, Porto Alegre, Brazil
- MP 161 **LC-MS/MS based absolute quantitation of hemoglobin subunits from DBS reveals novel biomarkers for α -thalassemia s**; Zhe Ren^{1,2}; Guoying Sun^{2,3}; Qianqian Zhang⁴; Shaomin Zou⁴; Jianhong Chen⁵; Weining Zhao⁶; Guixue Hou^{1,2}; Zeyan Zhong⁵; Jialong Li⁴; Yuhua Ye^{4,7}; Xiangmin Xu^{4,7}; Liang Lin^{1,2}; ¹BGI Genomics, BGI-Shenzhen, Shenzhen, China; ²Clinical laboratory of BGI Health, BGI-Shenzhen, Shenzhen, China; ³BGI Genomics, BGI-Shenzhen, Shenzhen, China; ⁴Department of Medical Genetics, School of Basic Medical Sciences, Southern Medical University, Guangzhou, China; ⁵Department of Medical Genetics and Prenatal Diagnosis, Huizhou First Maternal and Child Health Care Hospital, Huizhou, China; ⁶College of Pharmacy, Shenzhen Technology University, Shenzhen, China; ⁷Innovative Research Center for Diagnosis and Therapy of Thalassemias, Nanfang Hospital, Southern Medical University, Guangzhou, China
- MP 162 **Understanding the immunochemical mechanisms behind COVID-19 using a multi-OMIC, data independent mass spectrometry strategy**; Eleanor Matthews¹; Aishath Shaufa Shareef¹; Lee A Gethings²; Lisa Reid²; Adam King²; Stephen Fowler¹; Angela Simpson¹; Timothy Felton¹; Clare Mills³; ¹University of Manchester, Manchester, United Kingdom; ²Waters Corporation, Wilmslow, United Kingdom; ³University of Surrey, Guildford, United Kingdom
- MP 163 **Low picogram per mL Estrone quantitation in Serum at 8 Seconds per Sample Using the LDTD-MS/MS**; Serge Auger¹; Jean Lacourcière¹; Jonathan Rochon¹; Pierre Picard¹; ¹Phytronix Technologies, Quebec, QC
- MP 164 **Investigating the discriminatory potential of urinary DNA/RNA adductomics in head-neck cancers patients**; Sachin B Jorvekar¹; Aishwarya Jala¹; Sourabh Chouhan¹; Avdesh Rai²; Anupam Das³; Kaberi Kakati³; Kishore Das³; Anupam Sarma⁴; Roshan M Borkar¹; ¹National Institute of Pharmaceutical Education and Research-Guwahati, Guwahati, India; ²DBT Centre for Molecular Biology and Cancer Research, Dr. Bhubaneswar Borooh Cancer Institute, Guwahati, India; ³Department of Head and Neck Oncology, Dr. Bhubaneswar Borooh Cancer Institute, Guwahati, India; ⁴Department of Onco-Pathology, Dr. Bhubaneswar Borooh Cancer Institute, Guwahati, India
- MP 165 **Metabolite profiling applied to biomarker discovery in pancreatic cancer using high resolution LC-MS/MS**; Alan Barnes¹; Emily G Armitage¹; Neil Loftus¹; Elon Correa²; Lynne Howells³; Sèn Takeda⁴; Wen Chung⁵; ¹Shimadzu Corporation, Manchester, United Kingdom; ²Liverpool John Moores University, Liverpool, United Kingdom; ³Institute for Precision Health, The University of Leicester, Leicester, United Kingdom; ⁴Department of Anatomy, Teikyo University School of Medicine, Tokyo, Japan; ⁵Leicester HPB Unit, Glenfield Hospital, Leicester, United Kingdom
- MP 166 **Improving the stability of Alzheimer's disease plasma biomarkers: the impact of blood collection tubes with protease inhibitors**; Yijun Chen¹; Xuemei Zeng²; Carl Bertram¹; Thomas K Karikari¹; Nathan A Yates¹; ¹University of Pittsburgh, Pittsburgh, PA; ²University of Pittsburgh Medical Center, Pittsburgh, PA
- MP 167 **Mouse fatty liver proteomes in dda-PASEF and dia PASEF from low input using the timsTOF SCP**; Elizabeth Gordon¹; Matt Willetts²; Diego Assis³; Liwen Zhang⁴; Yanqiao Zhang⁵; ¹Bruker, Billerica, MA; ²Bruker Scientific, LLC, Billerica, MA; ³Bruker Scientific, Billerica, MA; ⁴Ohio State University, Columbus, OH; ⁵Northeast Ohio Medical University, Rootstown, OH 44272
- MP 168 **Temporal proteomic analysis of the high containment pathogen Ebola on primary human cells**; William Russell¹; Ruben Sota Acosta²; Lee K Palmer²; ¹University of Texas Medical Branch, Galveston, TX; ²UTMB at Galveston, Galveston, TX
- MP 169 **In Vivo Digestion Products of Dietary Gluten Proteins as Markers to Study Celiac Disease**; Jennifer A Sealey Voyksner¹; Robert Voyksner²; Jack Syage³; Chaitan Khosla⁴; Joseph Murray⁵; ¹ImmunogenX, Durham, NC; ²LCMS Limited, Durham, NC; ³ImmunogenX, Newport Beach, CA; ⁴Stanford University, Palo Alto, CA; ⁵Mayo Clinic, Rochester, MN
- MP 170 **Comparative analysis of extracellular vesicle low-molecular-weight proteins and peptides of cancer lines**; Aisha Sithika¹; Vivek Shekar¹; Adaikkalam Vellaichamy¹; ¹Anna University, Chennai, India
- MP 171 **Method Optimization of Cystine in urine as a Biomarker at 8 Seconds per Sample Using the LDTD-MS/MS Technique**; Jean Lacourcière¹; Serge Auger¹; Jonathan Rochon¹; Pierre Picard¹; ¹Phytronix Technologies, Quebec, QC
- MP 172 **High-content imaging and mass spectrometry-based drug screening platform to study stressor-induced tau aggregation**; Jie Xue^{1,2}; Long Cheng^{1,2}; Benoit Fatou^{1,2}; Mukesh Kumar^{1,2}; Kathrin Wenger^{1,2}; Arthur Viode^{1,2}; Hanno Steen^{1,2}; Judith Steen^{1,2}; ¹Boston Children's Hospital, Boston, MA; ²Harvard Medical School, Boston, MA
- MP 173 **Molecular characterization of inverse agonists targeting PPAR γ in bladder cancer using structural and quantitative proteomics**; Kuang-Ting Kuo^{1,2}; Ruben D. Garcia-Ordóñez³; Bilel Bdiri³; Theodore Kamenecka³; Patrick R. Griffin^{1,2,3}; ¹The Scripps Research, Jupiter, FL; ²Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; ³The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL
- MP 174 **Investigation of cellular response to the HSP90 inhibition in human cells through thermal proteome profiling**; Kejun Yin¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, GA
- MP 175 **Identification and separation of a major interference in the LC-MS/MS quantitative analysis of psilocin in mouse plasma**; Amir Khaiavinia¹; Deborah Michel¹; Randy W. Purves^{1,2}; Robert Laprarie¹; Anas El-Aneel¹; ¹University

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- of Saskatchewan, Saskatoon, SK; ²Canadian Food Inspection Agency, Saskatoon, SK
- MP 176 **Head-to-tail automation of covalent fragment screening and hit characterization by mass spectrometry for rapid lead discovery;** Jing Xue¹; Alexandra Frommlet¹; Robert Blake¹; Alexis Rohou¹; Melinda Mulvihill¹; Ke Sherry Li¹; ¹Genentech, South San Francisco, CA
- MP 177 **Covalent inhibitor screening of cellular protein targets using mass spectrometry for hit identification in living cells;** Sherry Ke Li¹; Ryan Conrad¹; Ryan Raisner¹; Brett Babin¹; Jing Xue¹; Melinda Mulvihill¹; ¹Genentech, South San Francisco, CA
- MP 178 **The Limited-Proteolysis method in Drug Development: Powerful workflow to identify drug targets and evaluate drug specificity;** Fabio Sabino¹; Jaruschka Pecnik¹; Roland Bruderer¹; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland
- MP 179 **Development and validation of an LC-MS/MS method for quantifying occidiofungin in rabbit plasma;** Andrew Cothrell¹; Ravi Orugunt²; James Leif Smith^{1,2}; ¹Texas A&M University, College Station, TX; ²Sano Chemicals, College Station, Texas
- MP 180 **Multiplexed CETSA MS as a tool for lead optimization;** Tuomas A Tolvanen^{1,2}; Jennifer A Amrhein³; Thomas Hanke³; Tomas Friman¹; Alexey Chernobrovkin¹; Stefan Knapp³; Michael Sundström²; Daniel Martinez Molina¹; ¹Pelago Bioscience AB, Solna, Sweden; ²Division of Rheumatology, Department of Medicine Solna, Karolinska University Hospital and Karolinska Institutet, Solna, Sweden; ³Institute of Pharmaceutical Chemistry, Goethe-University Frankfurt, Biozentrum, Frankfurt am Main, Germany
- MP 181 **Molecular Weight Determination and Sequence Confirmation of Oligonucleotides by LCMS-9030 Quadrupole Time-of-Flight (Q-TOF) Mass Spectrometer;** Xue Tang¹; Qiang Li²; Taohong Huang²; ¹Shimadzu?China?Co., Ltd., Chengdu, China; ²Shimadzu (China) Co., Ltd, Shanghai, China
- MP 182 **Measuring protein thermal stability and phosphorylation changes to capture early cellular responses to small molecule drugs;** Alexey Chernobrovkin¹; Daniel Martinez Molina¹; ¹Pelago Bioscience AB, Solna, Sweden
- MP 183 **Point-of-care quantitation of immunosuppressive drugs in blood by fast microextraction and miniature mass spectrometry analysis;** Yikun Liu¹; Jinling Lu¹; Wenpeng Zhang¹; Zheng Ouyang¹; ¹Tsinghua University, Beijing, China
- MP 184 **The Target Engagement Atlas - Mapping cell biology through small molecule perturbations;** Alexey Chernobrovkin¹; Tomas Friman¹; Erin Gilson¹; Bolette Bossen¹; Tuomas A Tolvanen¹; Daniel Martinez Molina¹; ¹Pelago Bioscience AB, Solna, Sweden
- MP 185 **Identification of Functionally Relevant and Druggable Protein Targets of Colorectal Cancer Chemoresistance using Protein Folding Stability Profiling;** Baiyi Quan¹; Morgan A. Bailey¹; John Mantyh²; Hsu S. Hsu²; Michael C. Fitzgerald¹; ¹Duke University, Durham, NC; ²Duke University Medical Center, Durham, NC
- MP 186 **Development and Optimization of an LC-MS/MS Method for CD73 Endogenous Biomarkers of Adenosine-5'-Monophosphate, Adenosine and Inosine;** Ashley Davie¹; Renmeng Liu¹; Yiding Hu¹; Ting Wang¹; Yurong Lai¹; ¹Gilead Sciences, Foster City, CA
- MP 187 **Mass Spectrometry Analysis with Cellular Thermal Shift Assay to Assess Senolytic Pathways in Senescent Monocytes;** Delaney Rutherford¹; Reema Banarjee¹; Quinn Strassheim¹; Amit K Dey¹; Dimitrios Tsitsipatis¹; Anjana Ram¹; Ruin Moaddel¹; Myriam Gorospe¹; Nathan Basisty¹; ¹National Institute on Aging, Baltimore, MD
- MP 188 **Validation of an Automated Process for the Determination of Covalent Modifier Potency: Kinact/KI of the Btk/Ibrutinib Model System;** William A Lamarr¹; Somayeh Talebzadeh¹; Jim Breunig²; Lars Hanson²; Brian Healey^{2,3}; ¹PureHoney Technologies, Inc., Billerica, MA; ²Beantown Biotech LLC, Billerica, MA; ³Revolution Biosciences LLC, Norwell, MA
- MP 189 **Characterization of Hyaluronic Acid-Based Hydrogel Drug Delivery Systems via Online Multimodal Liquid Chromatography-Mass Spectrometry;** Brady W Drennan¹; Kevin A. Schug¹; Sam H. Yang²; ¹University of Texas at Arlington, Arlington, TX; ²Genentech Inc, South San Francisco, CA
- MP 190 **Implementing antibody-free strategies for protein quantitation in monkey liver tissues using liquid chromatography coupled with mass spectrometry;** Yifan Shi¹; Sheng-Ping Wang¹; Lifeng Wang¹; Fritz Kramer¹; Wenying Jian¹; ¹Janssen Research & Development, Spring House, PA
- MP 191 **Rapid rank ordering of binding affinities of pools of test compounds against an RNA target with Affinity Selection Mass Spectrometry;** Somayeh Talebzadeh¹; Zane Thistleford¹; Can Jon Ozbal¹; ¹PureHoney Technologies, Billerica, MA
- MP 192 **The Neuropeptide Neuroparsin-A Regulates Caretaking Behavior in Leafcutter Ants;** Michael Gilbert¹; Karl Glastad¹; Maxx Fioriti Fioriti¹; Tierney Gannon¹; Matan Sorek¹; Lindsay Pino²; Shelley Berger¹; Benjamin A Garcia³; ¹University of Pennsylvania, Philadelphia, PA; ²Talus Bioscience, Seattle, WA; ³Washington University School of Medicine, St. Louis, MO
- MP 193 **Elucidating the mechanism of germline histone H3.3 mutations on neurodevelopment;** Elizabeth G. Porter¹; Francisca N. De Luna Vitorino¹; Khadija D. Wilson²; Yixuan (axe) Xie³; Peter Klein²; Elizabeth J. Bhoj²; Benjamin A. Garcia¹; ¹Washington University in St. Louis, St. Louis, MO; ²University of Pennsylvania, Philadelphia, PA; ³Washington University in St. Louis, St. Louis, MO
- MP 194 **Comprehensive interactome profiling of replication stress response and centromere instability by proximity labeling and affinity purification-mass spectrometry;** Alexander S. Lee^{1,2,3,4}; Basil B. Mattamana⁴; Justin E. Bodner^{1,2}; Renu Goel⁴; Daniel R. Foltz^{1,2}; Neil L. Kelleher^{1,2,3,4,5}; ¹Department of Biochemistry and Molecular Genetics, Northwestern University Feinberg School of Medicine, Chicago, IL; ²Simpson Querrey Institute for Epigenetics, Northwestern University, Chicago, IL; ³Chemistry of Life Processes Institute, Northwestern University, Evanston, IL; ⁴The Proteomics Center of Excellence, Northwestern University, Chicago, IL; ⁵Department of Chemistry and Molecular Biosciences, Northwestern University, Evanston, IL
- MP 195 **METTL3 Promotes Histone H3K9 Acetylation through Recruitment of Histone Acetyltransferase 1 to Chromatin;** Yen-Yu Yang¹; Xiaomei He¹; Jun Yuan¹; Chengjie Ma¹; Yinsheng Wang¹; ¹University of California Riverside, Riverside, CA
- MP 196 **Quantification of linker histone H1 proteoforms in naive versus germinal center B cells using capillary electrophoresis-top-down mass spectrometry;** Ashley Ives¹; Antonin Papin²; Alexey A. Soshnev³; Kevin Jooss¹; Navid Ayon¹; Matt Robey⁴; Ethel Cesarman²; Ari M. Melnick⁵; Rafael Melani¹; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL; ²Department of Pathology and Laboratory Medicine, Weill Cornell Medical College, New York, New York; ³Department of Neuroscience, Developmental and Regenerative Biology, University of Texas at San Antonio, San Antonio, Texas; ⁴Proteinaceous, Evanston, Illinois; ⁵Department of Medicine, Weill Cornell Medicine, New York, New York
- MP 197 **Top-down proteomics reveals proteoform changes in Histone H3.1 and H4 upon serum starvation of cells;** Jose A Villalobos¹; Nicolas L. Young¹; ¹Verna & Marrs McLean Department of Biochemistry & Molecular Biology, Baylor College of Medicine, Houston, TX

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- MP 198 **Histone proteoform quantitation uncovers the epigenetic response of brown adipose tissue to cold stress;** Bethany C Taylor¹; Allii M Nuotio-Antar¹; Nicolas L Young¹; ¹Baylor College of Medicine, Houston, Texas
- MP 199 **Scoring Post-translational Modification Crosstalk from Histone Proteoform Data;** Karl Fali Poncha¹; Nicolas L Young^{1,2,3}; ¹Verna and Marrs McLean Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX; ²Department of Molecular and Cellular Biology, Baylor College of Medicine, Houston, TX; ³Center for Precision Environmental Health, Baylor College of Medicine, Houston, TX
- MP 200 **Histone Post-Translational Modification Mapping of Aplysia californica Ganglia after Juvenile Exposure to Hypoxia using LC-TIMS-PASEF-ToF MS/MS;** Cassandra N. Fuller¹; Javier A. Rodriguez-Casariago^{2,3,4}; Lilian Valadares Tose¹; Jose M. Eirin-Lopez²; Lynne A. Fieber³; Francisco A. Fernandez-Lima¹; ¹Department of Chemistry and Biochemistry, Florida International University, Miami, FL; ²Department of Biology, Florida International University, Miami, FL; ³Department of Marine Biology and Ecology, Rosenstiel School, University of Miami, Miami, FL; ⁴Neurosciences Institute, University of Puerto Rico, San Juan, PR
- MP 201 **Quantitative Top-Down Analysis of H3.3K36M Oncohistone Proteoforms and Post-Translational Modifications;** Alyssa T. Paparella¹; Karl Poncha¹; Pratim Chowdhury¹; Ruhee Dere¹; Cheryl Lyn Walker¹; Nicolas L. Young¹; ¹Baylor College of Medicine, Houston, Texas
- MP 202 **"A Screening Method for the Determination of Atrazine in Aqueous and Lipid Based Foods by LC/MS";** Donna Payne¹; Sue D'Antonio²; Mike Adams³; Limian Zhao⁴; Anthony Macherone⁴; Greg Thompson⁴; ¹AnalytEval, SMITHVILLE, TX; ²Agilent Technologies, Cedar Creek, Texas; ³CWC Labs, Smithville, TX; ⁴Agilent Technologies, Wilmington, DE
- MP 203 **Automated Injection Solvent Modulation for Improved LC/MS Data Quality in the Measurement of Early Eluting Polar Pesticide;** Edgar Naegele; ^{Agilent Technologies, Waldbronn, Germany}
- MP 204 **Development of an LC-MS/MS Method for the Quantitation of Erythromycin A and Its Metabolites in Salmon Muscle;** Chaitali Chattopadhyaya; ^{FDA, CVM, Laurel, MD}
- MP 205 **Quantifying Insoluble Ferulic Acid and P-Coumaric Acid in Zea mays using LC-MS;** Valeria Zerda Pinto¹; Alayna Stephens¹; Cheyenne D Copling¹; Mary-Margaret B Benware¹; Tyson Lobb¹; David Buckley¹; Patrick S Carney¹; Hannah Labby¹; Fatima Romo¹; Carolyn J Butts-Wilmsmeyer¹; Kevin R Tucker¹; Olufunke M Ayegbidun¹; Ifeoluwa P Osikoya¹; Logan M Stenger²; Laura A Chatham²; Tiffany M Jamann²; Anthony J Studer²; Martin O Bohn²; Lucas M Roberts²; ¹Southern Illinois University Edwardsville, Edwardsville, IL; ²University of Illinois Urbana-Champaign, Urbana and Champaign, IL
- MP 206 **Investigation of Arsenic Accumulation in Deep-frying Oil;** Zhen-yan Li¹; Zhongping Yao²; ¹HK PolyU, Hung Hom, Hong Kong; ²HK PolyU, Hung Hom, Hong Kong
- MP 207 **Integrating veterinary drugs and pesticides into a targeted LC-MS/MS exposome-scale biomonitoring method;** Md Zakir Hossain¹; Yunyun Gu¹; Max Lennart Feuerstein^{1,2}; Benedikt Warth^{1,2}; ¹University of Vienna, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Währinger Straße 38, 1090, Vienna, Austria; ²Exposome Austria, Research Infrastructure and National EIRENE Hub, Vienna, Austria
- MP 208 **Simultaneous Determination of Neonicotinoids, Parabens, and Bisphenols in Canned Food Products by a Simplified QuEChERS and ID-UPLC-MS/MS;** Hsin-Chang Chen¹; Zou-Xiao Huang²; Jung-Wei Chang³; Po-Chin Huang^{4,5,6}; ¹Department of Chemistry, Tunghai University, Taichung City, Taiwan; ²Institute of Food Safety and Health, College of Public Health, National Taiwan University, Taipei, Taiwan; ³Institute of Environmental and Occupational Health Sciences, School of Medicine, National Yang Ming Chiao Tung University, Taipei, Taiwan; ⁴National Institute of Environmental Health Sciences, National Health Research Institutes, Miaoli, Taiwan; ⁵Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; ⁶Department of Medical Research, China Medical University Hospital, China Medical University, Taichung City, Taiwan
- MP 209 **Determination of nitrofuran metabolite residues in shrimp by LC-MS/MS;** Dan Luo¹; Qiang Li²; Hongyuan Hao³; Taohong Huang³; ¹Shimadzu (China) Co., LTD, Wuhan, China; ²Shimadzu (China) Co., LTD, Shanghai, China; ³Shimadzu (China) Co., Ltd, Shanghai, China
- MP 210 **Analysis of Antibiotics and Veterinary Drugs in Animal Feeds and Animal Tissues by QSight LC-MS/MS;** Jingcun Wu¹; Feng Qin¹; ¹PerkinElmer Inc., Woodbridge, ON
- MP 211 **Analysis of Residual Pesticides in Strawberries using the Quadrupole Time-of-Flight Mass Spectrometer;** Yuki Ito^{1,2}; Jun Watanabe^{1,2}; Junko Iida^{1,2}; ¹SHIMADZU Corporation, Kyoto, Japan; ²Osaka University Shimadzu Omics Innovation Research Laboratories, Suita, Japan
- MP 212 **Analysis of Veterinary Drugs in Chicken Tenders using the Quadrupole Time-of-Flight Mass Spectrometer;** Yuki Ito^{1,2}; Jun Watanabe^{1,2}; Junko Iida^{1,2}; ¹SHIMADZU Corporation, Kyoto, Japan; ²Osaka University Shimadzu Omics Innovation Research Laboratories, Suita, Japan
- MP 213 **Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Food Samples by LC-MS/MS;** Nozomi Maeshima¹; Ruth Marfil-Vega²; Manami Kobayashi¹; ¹SHIMADZU Corporation, Kawasaki, Japan; ²Shimadzu Scientific Instrument, Columbia, Maryland
- MP 214 **Development of high sensitivity and separation detection method for ciguatoxin analogues by LC/MS/MS;** Manami Kobayashi¹; Kaoru Nakagawa²; Ruth Marfil-Vega³; Junichi Masuda¹; Naomasa Oshiro⁴; ¹Shimadzu Corporation, Kawasaki-city, Japan; ²Shimadzu Corporation, Kyoto-city, Japan; ³Shimadzu Scientific Instruments, Columbia, MD; ⁴Division of Biomedical Food Research, National Institute of Health Sciences, Kawasaki-city, Japan
- MP 215 **Standard-Free Absolute Quantitation of Cyclic Imines using Tadem Mass Spectral Matching and LC/MRM-MS;** Nari Seo^{1,2}; Hee Young Jo^{1,2}; Hong Ju Kim^{1,2}; Myungjin Oh^{1,2}; Young Sang Kim³; You Jin Jeon³; Hyun Joo An^{1,2}; ¹Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; ²Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; ³Department of Marine Life Sciences, Jeju National University, Jeju-do, South Korea
- MP 216 **Automated sample preparation using CTC PAL3 to analyze >570 pesticides in orange by the combination of GC/MS/MS and LC/MS/MS techniques;** Zhiming Zhang¹; Ge Meng²; Zhicong Wang²; Jianguo Ji²; Chunxiao Wang²; ¹Agilent Technologies (Shanghai) Co., Ltd., Shanghai, China; ²Agilent Technologies, Shanghai, China
- MP 217 **Analysis of PAHs in Infant Formula with GC/MS with an EI Source Optimized for Use with Hydrogen Carrier Gas;** Jessica Westland¹; Limian Zhao¹; Bruce Quimby¹; Anastasia Andrianova¹; Lakshmi Krishnan²; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Santa Clara, CA
- MP 218 **Development of simplified LC-MS and LC-FAIMS-MS methods for the detection of gestagens in animal liver and fat;** Randy W Purves¹; Michelle West¹; Ratnadipsinh Vaghela¹; Jana Kinar¹; Yash Patel¹; Michael W Belford²; Bryn O. Shurmer¹; ¹Canadian Food Inspection Agency, Saskatoon, SK; ²Thermo Fisher Scientific, San Jose, CA
- MP 219 **Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Food Using a Novel Simplified Sample Preparation Method followed by LC/MS/MS Detection;**

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- MP 220 Limian Zhao¹; Matthew Giardina²; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Wilmington
Routine Pesticide Screening Solution: Data Independent Acquisition with a New LC/Q-TOF and Dedicated Screening Software; Cate Simmermaker¹; Christian Klein¹; Karen E Yannell¹; Kai Chen¹; Wei Wei¹; ¹Agilent Technologies, Santa Clara, CA
- MP 221 **Multi-Residue Pesticide Analysis in Cumin seeds using GC-MS/MS**; Durvesh Sawant¹; Rahul Dwivedi¹; Dr. Aseem Wagle¹; Prashant Hase¹; Sanket Chiplunkar¹; Hemant Kesarkar¹; Dr. Jitendra Kelkar¹; Dr. Pratap Rasam¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- MP 222 **Development of a search algorithm for rapid and accurate classification of edible oils by MALDI-MS**; Ho Yin Michael Ma¹; Suying Li¹; Zhongping Yao¹; ¹The Hong Kong Polytechnic University, Kowloon, Hong Kong
- MP 223 **Simplifying Dioxins Analysis in Foods and Feeds Using GC-MS/MS in Compliant with the EU Commission Regulation**; Rodrigo Ossamu Saga Kitamura¹; Adriana D'Agostinho²; Carolina Mariana Nunes²; Dereck Vitali Alves²; Roberta Oliveira Servilha²; ¹Shimadzu, Barueri, Brazil; ²Eurofins Special Tests, São Bernardo do Campo, Brazil
- MP 224 **Analytical method for multimycotoxin analysis in cereal grains using an Orbitrap Tribrid mass spectrometer**; Srinivas Sura¹; Micaela Gray¹; Jules Carlson¹; Xiben Wang¹; Maria Antonia Henriquez¹; ¹Agriculture and Agri-Food Canada, Morden, MB
- MP 225 **Achieving the MRLs with Hydrogen Carrier Gas: GC/MS/MS Analysis of 200 Pesticides in Produce**; Anastasia Andrianova¹; Eric Fausett¹; Bruce Quimby¹; Limian Zhao¹; Joel Ferrer²; Aaron Boice²; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Santa Clara, CA
- MP 226 **Determination of Over 500 Pesticides in Spice by EMR-GPD passthrough cleanup and a Novel Triple Quadrupole LC/MS system**; Hui Zhao¹; Linfeng Wu²; Limian Zhao¹; Patrick Batooon²; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Santa Clara, CA
- MP 227 **Ionic Liquid-Based Dispersive Liquid-Liquid Microextraction of Anthelmintic Drug Residues in caprine and ovine Meat Followed by LC-ESI-MS/MS Detection**; Rebagamang Tshepo¹; Simiso Dube¹; Mathew M Nindi¹; ¹UNISA, Florida Park, Rodepoort, South Africa
- MP 228 **Quantitation of N-nitrosamine impurities in dietary supplement by using LC-MS/MS**; Samruddha Chavan¹; Nitish Ramchandra Suryawanshi¹; Nitin Shukla¹; Nilesh Patil¹; Purushottam Sutar¹; Dr. Jitendra Kelkar¹; Dr. Pratap Rasam¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- MP 229 **Qualitative and Quantitative Characterization of Whiskey with Accurate Mass LC MS**; Sue D'Antonio¹; Nikolas Lau¹; Greg Thompson²; ¹Agilent Technologies, Cedar Creek, TX; ²Agilent Technologies, Wilmington, Delaware
- MP 230 **Determination of Famphur in Honey by Solid Phase Extraction and Gas Chromatography / Mass Spectrometry**; Seung-Woon Myung; ¹Kyonggi University, Suwon-Si, South Korea
- MP 231 **Nitrosation Dynamics of the Radical Cations of Guanine and Its Derivatives using Guided-Ion-Beam Tandem Mass Spectrometry**; Jonathan Benny¹; Jianbo Liu¹; ¹Queens College CUNY, Flushing, NY
- MP 232 **Secondary Proton Transfer during Ion/Ion Reactions between Metal-Adducted Peptides and Fluoranthene**; Darren Gass¹; Madeline G. Bannon¹; Michael S. Cordes¹; Sebastian N. Alberti¹; Elyssia S. Gallagher¹; ¹Baylor University, Waco, TX
- MP 233 **Reprogramming of ETD hardware control to enable ion-ion reactions between electrospray ions**; Jeff Brown¹; Richard Chapman¹; Emmy Hoyes¹; Sarah Brandner²; Frederik Lermyte²; ¹Waters Corporation, Wilmslow, United Kingdom; ²Technical University of Darmstadt, Darmstadt, Germany
- MP 234 **Sequencing of Phosphopeptide Anions via Sequential Charge Inversion Ion/Ion Reaction and Electron Capture Dissociation**; David V. Donndelinger¹; Xinheng Diao¹; Jonathan T. Specker¹; Tingting Yan¹; Boone M. Prentice¹; ¹University of Florida, Gainesville, FL
- MP 235 **Enhanced electron-anion interaction in electron-cation neutral plasma: Sequencing of oligonucleotides by electron-detachment dissociation**; Takashi Baba¹; Kaoru Karasawa²; Eva Duchoslav¹; ¹SCIEX, Concord, ON; ²AB SCIEX, Shinagawa, Japan
- MP 236 **Ion Parking in Native MS: Spectral Decongestion, Signal Concentration, and Mass Determination**; Nicolas J Pizzala¹; Scott A McLuckey²; Jay S Bhanot²; ¹Purdue University, West Lafayette, IN; ²Purdue University, WEST LAFAYETTE, IN
- MP 237 **Interaction of formates with proton-bound water complexes**; Malick Diedhioiu¹; Paul Mayer²; ¹University, Ottawa, ON; ²University of Ottawa, Ottawa, ON
- MP 238 **Dehydrogenations of Cyclohexane and Pyrrolidine by M(II) and M(O) Quinoline Complexes (M=Ni and Pd)**; Robert S King¹; Alexander Buzenski²; Richard A. J. O'hair³; Allan J Canty⁴; Victor Ryzhov⁵; ¹Northern Illinois University, DeKalb, IL; ²Northern Illinois University, DeKalb, IL; ³University of Melbourne, Melbourne, Australia; ⁴University of Tasmania, Hobart, Australia; ⁵Northern Illinois University (NIU), DeKalb, IL
- MP 239 **New Frontiers for Diserinol Isophthalamide as an Anion Complexation Reagent in Electrospray Ionization Mass Spectrometry**; Madeline Schultz¹; Sarah L. Parker¹; Maleesha T. Fernando¹; Miyuru M. Madduma Wellalage¹; Neil A. Ellis¹; Nwanne Dominic Banor¹; Daniel A. Thomas¹; ¹University of Rhode Island, Kingston, RI
- MP 240 **Charge Manipulation of Native Proteins via Gas-Phase Ion/Ion Reaction in a Tandem 2D-3D Digital Ion Trap Apparatus**; Liangxuan Fu¹; Scott A McLuckey¹; ¹Purdue University Department of Chemistry, West Lafayette, IN
- MP 241 **Gas-Phase Schiff Base Formation via PAMAM Dendrimer Molecular Containers**; Sarah Nsiah¹; Scott A McLuckey²; ¹Purdue University, West Lafayette, IN; ²Purdue University, WEST LAFAYETTE, IN
- MP 242 **Acidity of Organic Compounds and Small Peptides in Solution and in the Gas-Phase**; Kim Harvey¹; Mandy Brinkmann²; Michael Browne²; Erica Meng²; Raj Patel²; Jianhua Ren²; ¹University of the Pacific, Stockton, CA; ²University of The Pacific, Stockton, CA
- MP 243 **Selective, gas-phase decarboxylation of formic acid catalyzed by polyoxomolybdate anions**; Howard Z. Ma¹; Allan J. Canty²; Richard A. J. O'hair¹; ¹University of Melbourne, Parkville, Australia; ²University of Tasmania, Hobart, Australia
- MP 244 **Computational modelling of reaction intermediates in gas-phase charge inversion ion/ion reactions**; Yingchan Guo¹; Jonathan T. Specker¹; Ramón Alain Miranda-Quintana¹; Boone M. Prentice¹; ¹Department of Chemistry, University of Florida, Gainesville, FL
- MP 245 **Manipulation of gas-phase charge inversion ion/ion reaction reagents for kinetic and thermodynamic control over phospholipid identification in imaging mass spectrometry**; Jonathan T. Specker¹; Boone M. Prentice¹; ¹University of Florida Department of Chemistry, GAINESVILLE, FL
- MP 246 **Studies of Negative Electron Transfer Dissociation Reagents**; Keaton L Mertz¹; Katie Kothlow¹; Michael S. Westphall²; John E.P. Syka³; Joshua J. Coon²; ¹University of Wisconsin-Madison, Department of Chemistry, Madison, WI; ²University of Wisconsin-Madison, Madison, WI; ³Thermo Fisher Scientific, San Jose, California
- MP 247 **Chemical characterization of boron radical anions by studying gas-phase ion-molecule reactions in a mass spectrometer**; Jaskiran Kaur¹; Judy Kuan-Yu Liu²; Markus Rohdenburg³; Jonas Warneke³; Hilka I.

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- Kenttämäa¹; ¹Purdue University, West Lafayette, IN; ²Eli Lilly & Company, Indianapolis, IN; ³University of Leipzig, Leipzig, Germany
- MP 248 **Fragmentation Patterns of Peptoids Containing a Basic Residue**; Ashleigh Ramos¹; Yadwinder Singh Mann²; Jianhua Ren²; ¹University of the Pacific, Stockton, CA; ²University of The Pacific, Stockton, CA
- MP 249 **Structural elucidation of the 20S Proteasome using native ultraviolet photodissociation mass spectrometry**; Jada N. Walker¹; Amit Kumar Singh Gautam²; Andreas Matouschek^{2,3}; Jennifer S. Brodbelt¹; ¹Department of Chemistry, The University of Texas at Austin, Austin, TX; ²Department of Molecular Biosciences, The University of Texas at Austin, Austin, TX; ³Institute for Cell and Molecular Biology, The University of Texas at Austin, Austin, TX
- MP 250 **In-depth characterization of monoclonal antibody variants with native mass spectrometry**; Jun Dai¹; Chengjie Ji¹; ¹NovaBioAssays, Woburn, MA
- MP 251 **Size-Exclusion Chromatography-Native Mass Spectrometry Coupled with In-Source Denaturation Facilitates Characterization of Biologics for Drug Discovery**; Xiao Guo¹; Dongdong Wang¹; ¹Takeda Pharmaceuticals, Cambridge, MA
- MP 252 **Are Native Conformations of Proteins Preserved Throughout Laser Ablation?**; Neda Feizi Gilandeh¹; Blessing Chisom Egbejogun²; Kyle L. Wilhelm¹; Kermit K. Murray²; Touradj Solouki¹; ¹Baylor University, Waco, TX; ²Louisiana State University, Baton Rouge, LA
- MP 253 **Structural basis for allosteric modulation of the ABC transporter MsbA by copper(II) and lipid**; Jixing Lyu¹; Chang Liu²; Tianqi Zhang¹; Samantha Schrecke¹; Elam P. Nicklaus¹; Charles Packianathan¹; Georg K. A. Hochberg^{3,4}; David Russell¹; Minglei Zhao²; Arthur Laganowsky¹; ¹Texas A&M University, College Station, TX; ²University of Chicago, Chicago, IL; ³Max Planck Institute for Terrestrial Microbiology and Department of Chemistry, University of Marburg, Marburg, Germany; ⁴Center for Synthetic Microbiology (SYNMIKRO), Department of Chemistry, University of Marburg, Marburg, Germany
- MP 254 **Charge State Distributions of Proteins in Femto-Ampere ESI under Different pH**; Taoqing Wang¹; Huishan Li¹; Nicholas Allen¹; Ian T Ferraro¹; Anyin Li¹; ¹University of New Hampshire, Durham, NH
- MP 255 **Improving Ion Activation on a 1.5 m Fourier Transform Ion Mobility (FT-IM) Orbitrap using a Segmented Quadrupole Ion Trap**; Kacie Evans¹; Robert Schrader²; Carter Lantz²; David H. Russell²; ¹Texas A&M, College Station, TX; ²Texas A&M University, College Station, TX
- MP 256 **Quantitative Analysis of noncovalent Interactions via LILBID-MS**; Jonathan Schulte¹; Nina Morgner¹; Phoebe Young¹; ¹Goethe University Frankfurt, Frankfurt am Main, Germany
- MP 257 **Matrix-Landing Mass Spectrometry for Electron Microscopy Imaging of Native Protein Complexes**; Austin Z. Salome¹; Kenneth W. Lee¹; Timothy Grant¹; Michael S. Westphall¹; Joshua J. Coon¹; ¹University of Wisconsin-Madison, Madison, WI
- MP 258 **CDMS Analysis of Intact 19S, 20S, 26S, and 30S Proteasomes: Evidence for Higher-Order 20S Assemblies at low pH**; Adam J Anthony¹; Amit K. S. Gautam²; Lohra M. Miller¹; Anya G. Hardwick¹; Anu Sharma³; Subhadip Ghatak³; Andreas Matouschek²; Martin F. Jarrold¹; David E. Clemmer¹; ¹Indiana University, Bloomington, IN; ²Department of Molecular Biosciences, Austin, TX; ³Indiana Center for Regenerative Medicine and Engineering, Department of Surgery, Indianapolis, IN
- MP 259 **An Evaluation of Ion Mobility-Collision Induced Unfolding (IM-CIU) Methods Leveraging Cyclic Ion Mobility Separation for the Evaluation of Protein Dynamics**; Addison E. Bergman¹; Devin M. Makey¹; Ryan Schroeder¹; Brandon T. Ruotolo¹; ¹University of Michigan, Ann Arbor, MI
- MP 260 **Improved Signal Processing for Orbitrap Charge Detection Mass Spectrometry**; Michael Goodwin¹; Kyle Patrick Bowen¹; Dmitry Grinfeld¹; Ping Yip¹; Michael Senko¹; ¹Thermo Fisher Scientific, San Jose, CA
- MP 261 **Fluorinated ethylamines as ESI-friendly neutral pH buffers for native mass spectrometry**; Brad Davis¹; Algirdas Velyvis¹; Siavash Vahidi¹; ¹University of Guelph, Guelph, ON
- MP 262 **Towards understanding the effect of isoelectric point on the gas-phase stability of proteins in native MS**; Alexis N. Edwards¹; Michael S. Cordes¹; Elyssia S. Gallagher¹; ¹Baylor University, Waco, TX
- MP 263 **Native ESI MS for Deep Characterization of Target Engagement and Molecular Mode of Action**; Xidong Feng¹; Wenyi Hua²; Jayasankar Jasti²; Timothy Foley²; Dafydd Owen²; Matthew D Troutman²; ¹Pfizer, Groton, CT; ²Pfizer Inc., Groton, CT
- MP 264 **Multiplexed interrogation of selective inhibitors of fatty acid-binding proteins by native mass spectrometry**; Michelle Q Phan¹; Indu R Chandrashekar^{1,2}; Naureen Akhtar^{1,2}; Evgenia Konstantinidou^{1,2}; Thomas Nebel³; Darren J Creek⁴; Martin J Scanlon^{1,2}; Raymond S Norton^{1,2}; ¹Medicinal Chemistry, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Australia; ²ARC Centre for Fragment-Based Design, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Australia; ³Biology Group, Biomedical Manufacturing Program, CSIRO, Clayton, Australia; ⁴Drug Delivery, Disposition and Dynamics, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Australia
- MP 265 **Native MS for gas-phase metallochemistry of amyloid β** ; Sarah Brandner¹; Tanja Habeck¹; Frederik Lermyte¹; ¹TU Darmstadt, Darmstadt, Germany
- MP 266 **Exploring Nonannular Belt of Membrane Proteins Using Charge Reduction**; Smriti Kumar; Texas A&M University, College Station, TX
- MP 267 **Assessment of Monoclonal Antibody Structure, Stability, and Developability using Native LC-MS**; Yu Zhou¹; Jakub Baudys²; Ryan Li³; Theodore R. Keppel¹; Sarah H. Osman²; Christopher A. Haynes¹; John R Barr¹; Dongxia Wang¹; ¹Center for Disease Control and Prevention, Atlanta, GA; ²Centers for Disease Control and Prevention, Atlanta, GA; ³Augusta university, Augusta, Georgia
- MP 268 **Characterization of protein - protein and protein - ligand interactions by tandem-trapped ion mobility spectrometry/mass spectrometry and structure relaxation approximation**; Fanny C Liu¹; Tyler C Cropley¹; Olufemi Araoyinbo¹; Christian Bleiholder¹; ¹Florida State University, Tallahassee, FL
- MP 269 **Expanding glycoproteome analysis with Activated-Ion ETD on an Orbitrap Ascend Tribrid**; Annie Jen¹; Trenton M. Peters-Clarke²; Yuchen He¹; Keaton L. Mertz²; Evgenia Shishkova^{1,3}; Michael S. Westphall¹; Joshua J. Coon^{1,2,3,4}; ¹Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI; ²Department of Chemistry, University of Wisconsin - Madison, Madison, WI; ³National Center for Quantitative Biology of Complex Systems, Madison, WI; ⁴Morgridge Institute for Research, Madison, WI
- MP 270 **False positive glycopeptide identification through in-FAIMS glycan fragmentation**; Valentina Rangel Anzarita¹; Keira E. Mahoney¹; Catherine Kwon¹; Raibat Sarker¹; Stacy A. Malaker¹; ¹Yale University, New Haven, CT
- MP 271 **High Abundance Protein Depletion Combined with Isobaric Tag Boosting Expands N-glycoproteome Coverage in Serum Samples**; Jingwei Zhang¹; Yuan Liu¹; Danqing Wang¹; Zicong Wang¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- MP 272 **A Mass Spectrometry-Based Chemical and Enzymatic Method to Comprehensively Analyze Protein O-**

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- MP 273 **GlcNAcylation and O-GalNAcylation**; Senhan Xu¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, GA
- MP 274 **Combining selective enrichment and a boosting approach to globally and site-specifically characterize protein co-translational O-GlcNAcylation**; Senhan Xu¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, GA
- MP 275 **Anion exchange chromatography-mass spectrometry to characterize alpha-1-acid glycoprotein proteoforms and monitor changes during pregnancy**; Guusje Van Schaick¹; Manfred Wuhrer¹; Elena Dominguez Vega¹; ¹Center for Proteomics and Metabolomics, LUMC, Leiden, Netherlands
- MP 276 **Spike Glycoprotein S1 Site-specific O-glycosylation: Systematic and Comparative Analysis from Eleven Variants of SARS CoV-2**; Sherifdeen B Onigbinde¹; Cristian D Gutierrez Reyes¹; Mojibola O Fowowe¹; Oluwatosin E Daramola¹; Mojgan Atashi¹; Andrew I. Bennett¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- MP 277 **Quantification of the glycoproteome and surfaceome dynamics during epithelial-to-mesenchymal transition (EMT)**; Xing Xu¹; Kejun Yin¹; Zeyu Wang¹; Ronghu Wu¹; ¹Georgia Institute of Technology, Atlanta, GA
- MP 278 **MRM analysis of glycosyltransferases in fibroblasts of CDG patients**; Andreas Harst¹; Cedric Stahl²; Nicole Luebbhusen¹; Ute Bach¹; Roman Sakson³; Christian Thiel²; Thomas Ruppert¹; ¹Zentrum fuer molekulare Biologie Heidelberg, Universitaet Heidelberg, Heidelberg, Germany; ²Heidelberg University Hospital, Heidelberg, Germany; ³University of applied Science, Mannheim, Germany
- MP 279 **Global analysis of site-specific glycosylation in serum reveals novel candidate biomarker pattern with atypical N-glycosites for diagnosis of hepatocellular carcinoma**; Siyuan Kong¹; Weiqian Cao¹; ¹Institutes of Biomedical Sciences, Fudan University, Shanghai, China
- MP 280 **LC-MS/MS Quantitation of HILIC-Enriched N-glycopeptides derived from low abundance serum glycoproteins in patients with Narcolepsy Type 1**; Mojgan Atashi¹; Cristian D Gutierrez Reyes¹; Vishal Sandilya¹; Waziha Purba¹; Parisa Ahmadi¹; Akeem Adeyemi Sanni¹; Zihan Monshad¹; Firas Kobeissy²; Giuseppe Plazzi³; Raffaele Ferri⁴; Yehia Mechref¹; ¹Texas Tech University, Lubbock; ²Morehouse School of Medicine (MSM), Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Atlanta, Georgia; ³Department of Biomedical, Metabolic and Neural Sciences, University of Modena and Reggio Emilia, Modena, Italy; ⁴Sleep Research Centre, Department of Neurology IC, Oasi Research Institute- IRCCS, Troina, Italy
- MP 281 **Identifying glycan site profile differences of CD33 expressed in HEK293 and CHO cells**; Kyle Hoffman; ¹Bioinformatics Solutions Inc, Waterloo
- MP 282 **Investigation of glycosylation of CD209L/L-SIGN and CD209/DC-SIGN and their features as receptors for SARS-CoV-2 infection**; Chaoshuang Xia¹; Nader Rahimi¹; Catherine E. Costello¹; ¹Boston University Chobanian and Avedisian School of Medicine, Boston, MA
- MP 283 **Identifying Conserved Glycoproteomic Alterations in Clinical Samples and Animal Models of Ureteropelvic Junction Obstruction**; John Froehlich^{1,2}; George Lambrinos¹; Shannon Dimartino¹; Alexander Bigger-Allen^{1,2}; Rosalyn Adam^{1,2}; Richard Lee^{1,2}; ¹Children's Hospital Boston, Boston, MA; ²Harvard Medical School, Boston, MA
- MP 284 **Mass Spectrometry Analysis of Intact Glycopeptides in Human Clear Cell Renal Cell Carcinoma Tissue Samples**; Fernando Garcia-Marques¹; Abel Bermudez¹; Hongjuan Zhao²; Rosalie Nolley²; James D Brooks²; Sharon J Pitteri¹; ¹Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; ²Department of Urology, Stanford University School of Medicine, Stanford, CA
- MP 285 **COVID Spike protein functions are modulated by disulfide linkage patterns. Considerations for vaccine development**; Andrew D Mahan¹; Alexander N Barnakov²; Hirsh Nanda²; ¹Johnson and Johnson, Spring House, PA; ²Johnson & Johnson, Spring House, PA
- MP 286 **In-depth Characterization of Heterogeneity in Glycoproteoform by Individual Ion Mass Spectrometry (I2MS) and I2MS2**; Jua Lee¹; Taojunfeng Su¹; Pei Su¹; John P. McGee¹; Steven M. Patrie¹; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL
- MP 287 **Mapping Low Abundant Serum Glycoproteome Using Ranachrome-5 Immobilized Magnetic Terpolymer as a Super HILIC Sorbent for Hepatocellular Carcinoma Biomarker Discovery**; Muhammad Salman Sajid¹; Habtom Resson¹; ¹Georgetown University, Washington, DC
- MP 288 **Combining orthogonal glycan analysis techniques for a deeper understanding of a tri-specific protein**; Michael McKinnon; ¹Novartis Institutes for Biomed. Research, Inc., Cambridge, MA
- MP 289 **Hybrid LBA-LC-MS/MS method for glycan-resolved PK monitoring of a therapeutic fusion protein**; Ines C Santos¹; Brian Melo¹; Linna Wang¹; Yury Chaly¹; Bonnie Wang¹; Yongjun Xue¹; Jim Shen¹; Sekhar Surapaneni¹; ¹Bristol Myers Squibb, Princeton, NJ
- MP 290 **New HPLC column for the fast analysis of carbohydrates and glycans by LC-MS**; Hendrik-Jan Brouwer¹; Jean-Pierre Chervet¹; Christian Marvelous¹; Thijs Mulder¹; Martin Eysberg²; ¹Antec Scientific, Alphen a/d Rijn, Netherlands; ²Antec Scientific, Boston, MA 02108
- MP 291 **Unraveling the Released N-Glycan Complexity by Implementing High-Resolution Ion Mobility in the HILIC-MS Workflow**; Jordan Stewart¹; Brandon Nelson¹; Shahadat Reza¹; Heidi Vitrac¹; ¹MOBILion Systems, Inc., Chadds Ford, PA
- MP 292 **Rapid CE-MS analysis of released N-glycan: optimized workflow for direct CE compatibility**; Patrice Knightly¹; Sara Carillo¹; Adi Kulkarni²; Erin Redman²; Catherine Rawlins²; Kate Yu²; Jonathan Bones¹; ¹National Institute of Bioprocessing Research and Training, Dublin, Ireland; ²908 Devices, Boston, MA
- MP 293 **Comprehensive N-glycan Profiling of USP Monoclonal Antibody Reference Standard using GlycanExplorerTMS Software**; Arun Apte¹; Rupanjan Goswami¹; Karthik Kolli¹; ¹PREMIER Biosoft, San Francisco, CA
- MP 294 **Characterization of Bile-Salt Stimulated Lipase and Mucin O-glycopeptides by Different Dissociation Techniques**; Joy O Solomon¹; Sherifdeen B Onigbinde¹; Cristian D Gutierrez Reyes¹; Mojibola O Fowowe¹; Oluwatosin E Daramola¹; Andrew I. Bennett¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, Texas
- MP 295 **Application of acoustic ejection coupled to high-resolution mass spectrometry (AE-HRMS) to Metabolite Identification Studies**; Alandra Quinn¹; Chang Liu²; Gordana Ivosev²; Carley Heck¹; Dennis Hyek¹; George Hajj¹; Brendon Kapinos¹; Usa Reilly¹; ¹Pfizer, Groton, CT; ²SCIEX, Concord, ON
- MP 296 **Increasing sensitivity of high throughput host cell protein analysis on a novel high-resolution accurate mass platform**; Eugen Damoc¹; Tabiwang N. Arrey¹; Anna Pashkova¹; Eduard Denisov¹; Kai Scheffler²; Kristina Srzentic³; ¹Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ²Thermo Fisher Scientific, Germering, Germany; ³Thermo Fisher Scientific, Reinach, Germany
- MP 297 **Single-shot LC-MS workflow for comprehensive proteome identification on a novel high-resolution accurate mass platform**; Santosh Renuse¹; Tabiwang N. Arrey²; Anna Pashkova²; Maowei Dou³; Jeff Op De Beeck⁴; Ryan Bomgarden³; Bernard Delanghe²; Eugen Damoc²; Sally Webb¹; ¹ThermoFisher Scientific, San Jose, CA; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ³Thermo Fisher Scientific, Rockford, IL; ⁴Thermo Fisher Scientific, Ghent, Belgium
- MP 298 **Targeted Whole-Pathway Proteomic Assays with Sample Multiplexing: Data Visualization-Guided Optimization**; Steven R. Shuken¹; Devin K. Schweppe^{1,2};

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- Xinyue Liu¹; Joao A. Paulo¹; Steven P. Gygi¹; Qing Yu¹;
¹Department of Cell Biology, Harvard Medical School, Boston, MA; ²Department of Genome Sciences, University of Washington, Seattle, WA
- MP 298 **Developing a Semi-Automated Sample Preparation Method for the Enrichment of Biotinylated Proteins; Noah Smeriglio¹; Ashley Frankenfield¹; Haorong Li¹; Jiawei Ni¹; Ling Hao¹; ¹Department of Chemistry, George Washington University, Washington, DC**
- MP 299 **Screening Clones for Monoclonal Antibody Production Using Droplet Microfluidics Interfaced to Electrospray Ionization Mass Spectrometry; Cara I D'amico¹; Gillian E. Robbins²; Iris Po³; Zichao Fang³; Thomas R. Slaney³; Li Tao³; Gabi Tremml³; Brandon T. Ruotolo²; Robert T. Kennedy²; ¹Bristol Myers Squibb, Summit, NJ; ²University of Michigan, Ann Arbor, MI; ³Bristol Myers Squibb, New Brunswick, NJ**
- MP 300 **RTMS: An R Toolkit for Extracting, Analyzing, and Visualizing High-Throughput MALDI Mass Spectrometry Data; Mary Ashley Rimmer¹; Nathaniel R Twarog¹; John Bowling¹; Brandon Young¹; Anang A Shelat¹; Zoran Rankovic¹; ¹St. Jude Children's Hospital, Memphis, TN**
- MP 301 **High-throughput Late-stage Synthesis of Complex Bioactive Molecules by Desorption Electrospray Ionization Mass Spectrometry (DESI-MS); Kai-Hung Huang¹; Nicolas M. Morato¹; Veronica Feng¹; Eric T. Dziekonski¹; R. Graham Cooks¹; ¹Purdue University, WEST LAFAYETTE, IN**
- MP 302 **Multiplex analysis of bile acids using isobaric labeling with triple quadrupole mass spectrometry; Suzumi M Tokuoka¹; Yoshiya Oda¹; ¹The University of Tokyo, Tokyo, Japan**
- MP 303 **High-throughput and low-volume analysis of native and intact protein mixtures with LAP-MALDI MS; Bob Challen¹; Mike Morris²; Rainer Cramer¹; ¹University of Reading, Reading, United Kingdom; ²Waters Corporation, Wilmslow, United Kingdom**
- MP 304 **Fast Quantification of essential amino acids in plasma using LDTD-MS/MS; Francis Briere^{1,2}; Jacques Corbeil^{1,2,3}; Serge Auger⁴; ¹Centre Nutriss, INAF, Université Laval, Québec, Qc; ²CHU de Québec, Université Laval, Québec, Qc; ³Big Data Research Center, Québec, Qc; ⁴Phytronix Technologies Inc., Quebec, CA**
- MP 305 **Introducing ion mobility spectrometry for rapid LC-MS: Validation and its application to large scale human blood sample sets; Yoshihiro Kita¹; Suzumi M Tokuoka¹; Georgis Isaac²; Lee A Gethings³; Robert S Plumb²; Yoshiya Oda¹; ¹The University of Tokyo, Tokyo, Japan; ²Waters Corporation, Milford, MA; ³Waters Corporation, Wilmslow, United Kingdom**
- MP 306 **Simultaneous Multi-Omics by Direct Infusion Mass Spectrometry (SMAD-MS); Yuming Jiang¹; Jesse Meyer²; ¹ceders-sinai medical center, Los Angeles, CA; ²Cedars-Sinai Medical Center, Los Angeles, CA**
- MP 307 **Snapshots of the Membrane: A high-throughput proteomic screen capturing membrane proteins in their native environment for structural and functional studies; Caroline Brown^{1,2}; Snehasish Ghosh^{1,2}; Yansheng Liu^{3,4}; Moitrayee Bhattacharyya³; Kallol Gupta^{1,2}; ¹Nanobiology Institute, Yale University, West Haven, Connecticut; ²Yale School of Medicine, Department of Cell Biology, New Haven, CT; ³Yale School of Medicine, Department of Pharmacology, New Haven, CT; ⁴Cancer Biology Institute, West Haven, CT**
- MP 308 **Incorporating Ferrimagnetic Beads to High Throughput Affinity Selection Mass Spectrometry; Jonathan Shrimp¹; Nate Hoxie¹; John Janiszewski¹; Colin Kelly¹; Matthew Hall¹; Sam Michael¹; Meghav Verma¹; Anton Simeonov¹; Michael Ronzetti¹; Bolormaa Baljinnyam¹; Thomas R. Covey²; Peter Kovarik²; Chang Liu²; Richard Van Breenen³; Jianli Zhao⁴; Emmet Welch⁴; Sasikumar Pillai⁵; Subhasish Purkayastha⁵; ¹NCATS/NIH, Rockville, MD; ²SCIEX, Concord; ³Oregon State University, Corvallis, OR; ⁴Phenomenex, Torrance, CA; ⁵Sciex, Framingham, MA**
- MP 309 **All-in-One Design and Analysis of Quantitative Studies for High Throughput Experiments; Richard Lee¹; Nikki Dare¹; Nikolay Malashchenok¹; Karl Demmans¹; ¹ACD/Labs, Toronto, ON**
- MP 310 **Fully-integrated, high-throughput, dual-stream microflow LC-MS/MS for in vitro screening bioanalysis; Jamie R Kirsch¹; Jillian Racich¹; Daria Vernikovskaya¹; Brendon Kapinos¹; Anthony Carlo¹; Wayne Lootsma²; Steve Ainley²; ¹Pfizer Inc., Groton, CT; ²Sound Analytics, Niantic, CT**
- MP 311 **Ultra-fast Online SPE Applicable to a Wide Range of Compounds with Various Hydrophobicity for High-throughput Analysis using Multiplexed 4-channel 2D-LC-MS/MS; Eishi Imoto¹; Toshiya Matsubara¹; ¹Shimadzu Scientific Instruments, Columbia, MD**
- MP 312 **Ultra-High-Throughput Compound Quality Control with Acoustic Ejection Mass Spectrometry; Chang Liu¹; Alandra Quinn²; Gordana Ivosev¹; Robert Mongillo²; Bhagyashree Khunte²; Brendon Kapinos²; ¹SCIEX, Concord, ON; ²Pfizer, Groton, CT**
- MP 313 **Desorption enhancing solution optimization for High-Throughput screening of 1536 samples at 0.96 Seconds per Sample Using the LDTD-HTS-MS/MS; Pierre Picard¹; Serge Auger¹; Jean Lacourcière¹; Jonathan Rochon¹; ¹Phytronix Technologies, Inc., Quebec, QC**
- MP 314 **High Throughput Screening via Ambient Ionization 2D MS/MS for Discovery of Medical Countermeasures Against New and Emerging Threats; Andy Eller¹; Mitch Wells¹; Dalton Snyder¹; Anna Leech¹; Ann Donnelly¹; Miranda Jacobs¹; Jennifer Poole¹; ¹Teledyne FLIR, West Lafayette, IN**
- MP 315 **A Real-time Informatics Pipeline Enables Screening of Biologics during High-Throughput Expression; Xianqin Zhai¹; Behnam Keshavarz²; Sidharth Mohan²; Bo Zhai²; Elsa Gorre²; Jing Li¹; Andrew Mahan²; Iman Farasat²; Hirsh Nanda²; Marshall Bern¹; Harsha Gunawardena²; ¹Protein Metric Inc., Cupertino, CA; ²JOHNSON AND JOHNSON, Spring House, PA**
- MP 316 **Coupling online buffer exchange with automated data processing for screening designed protein complexes by native mass spectrometry; William Resager¹; Marius M Kostelic²; Vicki H Wysocki²; Marshall Bern¹; ¹Protein Metrics, LLC, Cupertino, CA; ²Ohio State University, Columbus, OH**
- MP 317 **Rapid Identification of Changes of Small Molecules in MALDI-MSI Data of Tumor Spheroids; Yijia Wang¹; David Hua²; Heather Desaire²; Amanda B Hummon¹; ¹The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; ²University of Kansas, Department of Chemistry, Lawrence, KS**
- MP 318 **METASPACE-ML: A machine-learning approach for annotating metabolites and lipids in imaging mass spectrometry data; Bishov W Abdelmalak¹; Lachlan Stuart^{1,2}; Måns Ekelöf¹; Sergii Mamedov¹; Lucas Maciel Vieira¹; Theodore Alexandrov^{1,3,4,5}; ¹Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany; ²EMBL, Heidelberg, Germany; ³Metabolomics Core Facility, Heidelberg, Germany; ⁴Molecular Medicine Partnership Unit, Heidelberg, Germany; ⁵Bio Studio, BiInnovation Institute, Copenhagen, Denmark**
- MP 319 **Ion-to-image (i2i) – a new application for unique and rapid processing of mass spectrometry imaging data; Johan Lillja¹; Kyle D. Duncan^{1,2}; Ingela Lanekoff³; ¹Uppsala University, uppsala, Sweden; ²Vancouver Island University, Nanaimo, BC; ³Uppsala University, Uppsala, Sweden**
- MP 320 **iFAMS Imager: A Streamlined Gábor Deconvolution Workflow for Mass Spectrometry Imaging, Protein Localization, and Heatmap Cross-Comparison; Lily E Miller¹; Andrew K Swansiger¹; Manxi Yang²; Julia Laskin²; James S Prell^{1,3}; ¹University of Oregon, Eugene, OR;**

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- MP 321 ²Purdue University, WEST LAFAYETTE, IN; ³Materials Science Institute, University of Oregon, Eugene, OR
Identifying Colocalized Compounds in Mass Spectrometry Images of Diverse Tissue Samples Using Unsupervised Deep Learning; Emerson Hernly¹; Rosemary Ajish¹; Julia Laskin¹; ¹Purdue University, West Lafayette, IN
- MP 322 **Low-Rank Modeling with Sparse and Dense Residuals Enables Advanced Dimensionality Reduction for Imaging Mass Spectrometry Measurements of Human Eye Tissue;** Roger A.R. Moens¹; Lukasz G Migas¹; David Anderson²; Christine A. Curcio³; Richard M Caprioli^{2, 4, 5, 6, 7}; Kevin Schey^{2, 4}; Jeffrey M Spraggins^{2, 4, 5, 8}; Raf Van De Plas^{1, 2, 4}; ¹Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ²Department of Biochemistry, Vanderbilt University, Nashville, TN; ³Department of Ophthalmology and Visual Sciences, University of Alabama at Birmingham, Birmingham, AL; ⁴Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ⁵Department of Chemistry, Vanderbilt University, Nashville, TN; ⁶Department of Medicine, Vanderbilt University, Nashville, TN; ⁷Department of Pharmacology, Vanderbilt University, Nashville, TN; ⁸Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN
- MP 323 **Enhancing Spatial Resolution in Tandem Mass Spectrometry Ion/Ion Reaction Imaging Experiments through Image Fusion using Convolutional Neural Networks;** Xizheng (colin) Diao¹; Zhongling Liang¹; Yingchan Guo¹; Boone M. Prentice¹; ¹University of Florida, Gainesville, FL
- MP 324 **A multi-modal image fusion workflow incorporating MALDI imaging mass spectrometry and microscopy for the study of small pharmaceutical compounds;** Zhongling Liang¹; Abhishek Sharma²; Christopher R. McCurdy²; Boone M. Prentice¹; ¹University of Florida Department of Chemistry, GAINESVILLE, FL; ²College of Pharmacy, University of Florida, Gainesville, FL
- MP 325 **From Spectra to Molecules in Spatial Metabolomics: Data processing and metabolite annotation of AP-SMALDI-Orbitrap data using METASPACE;** Domenic Dreisbach¹; Carolin M Morawietz²; Theodore Alexandrov³; Bernhard Spengler^{1, 2}; Kerstin Strupat⁴; ¹TransMIT GmbH, Giessen, Germany; ²Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Germany; ³European Molecular Biology Laboratory, Heidelberg, Germany; ⁴Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- MP 326 **A data interpretation workflow for the analysis of peptides from complex atmospheric pressure MALDI mass spectrometry histochemistry (MSHC) imaging datasets;** Nivedita Bhattacharya^{1, 2, 3}; Kenneth Verheggen²; Konstantin O. Nagornov⁴; Yury O. Tsybin⁴; Peter D. Verhaert²; ¹MassTech, Columbia, MD; ²ProteoFormix, Beerse, Belgium; ³Barefeet Analytics Private Limited, Pune, India; ⁴Spectroswiss, 1015, Lausanne, Switzerland
- MP 327 **Are biological mass spectrometry imaging (MSI) studies sufficiently powered? Measurement and characterisation of uncertainty in mass spectrometry imaging experiments;** Alexander Dexter¹; Felicia Wirtz¹; Rory Thomas Steven¹; Caroline Pollard¹; Lily Ellis-Gibbings¹; Stephanie Ling²; Richard J A Goodwin²; Simon T Barry²; Josephine Bunch^{1, 3}; ¹National Physical Laboratory, Teddington, United Kingdom; ²AstraZeneca, Cambridge, United Kingdom; ³Imperial College, London, London, United Kingdom
- MP 328 **Innovative Software Solutions for Measuring Analyte Delocalization in MALDI Imaging;** Cole C Johnson¹; Dalton R Brown¹; Caitlin M. Tressler¹; Nathan Riemann¹; Jason Fan¹; Kristine Glunde¹; ¹Johns Hopkins School of Medicine, Baltimore, MD
- MP 329 **Pixel-to-pixel metabolite ratio imaging as a novel tool to advance pathway analysis in MALDI MS Imaging studies;** Joshua L Fischer¹; Ethan Yang¹; Dawson Miller²; Steven S Gross²; Qiuying Chen³; ¹Bruker Scientific, LLC, Billerica, MA; ²Weill Cornell Medicine, New York, NY; ³Cornell University Medical College, New York, NY
- MP 330 **Statistical Heterospectroscopy of MALDI Imaging and NMR Spectroscopy Data for Evaluation of Breast Tumor Models;** Dalton Brown¹; Caitlin M. Tressler^{1, 2}; Cole Johnson¹; Sophia Nakuchima¹; Ethan Yang^{1, 2}; Kristine Glunde^{1, 2}; ¹Johns Hopkins AIMS Core, Baltimore, MD; ²Johns Hopkins School of Medicine, Baltimore, MD
- MP 331 **Metabolite database searching tool in MSiReader for mass spectrometry imaging annotations;** Cristina Arciniega¹; Tana Palomino¹; Alexandria L. Sohn¹; Mary F. Wang¹; David C Muddiman¹; ¹NCSU, Raleigh, NC
- MP 332 **Clustering of mass spectrometry imaging data without dimensionality reduction;** Stanislav Pekov^{1, 2, 3}; Mariya Derkach²; Anatoly Sorokin^{2, 4}; Mariya Shamraeva²; Eugene (evgeny) Nikolaev¹; Igor Popov²; ¹Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; ²Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation; ³Siberian State Medical University, Tomsk, Russia; ⁴Okinawa Institute of Science and Technology, Onna, Japan
- MP 333 **MSI Quantify: A micro-app for the automated processing of quantitative mass spectrometry imaging data;** Scott Trinkle¹; Emmanuelle Claude²; Emrys Jones²; Mark Towers²; Richard Chapman¹; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Wilmslow, United Kingdom
- MP 334 **Automated visualization, exploration and material segmentation of ion-mobility mass spectrometry imaging data;** Scott Trinkle¹; Ayushe Gangal¹; Joanne Mather¹; Bindesh Shrestha¹; Richard Chapman¹; ¹Waters Corporation, Milford, MA
- MP 335 **An automated workflow for combining, aligning, exploring, and visualising 3D MS imaging data;** Richard Chapman¹; Scott Trinkle¹; Emrys A Jones²; ¹Waters, Milford, MA; ²Waters, Wilmslow, United Kingdom
- MP 336 **Developing an Expansion Protocol to Improve Spatial Resolution in Mass Spectrometry Imaging;** Li-Cyun Chen¹; Cheng-Chih Hsu¹; Chuping Lee²; ¹Cheng-Chih Richard Hsu Lab, Department of Chemistry, National Taiwan University, Taipei City, Taiwan; ²National Chung Hsing University, Taichung, Taiwan
- MP 337 **Development of a novel analytical method for monitoring individual health status using mass spectrometry imaging of hair samples;** Shuichi Shimma^{1, 2}; Hiromi Saito¹; Erika Nagano²; Kazuki Odake²; ¹Osaka University, Suita, Osaka, Japan; ²Miruion inc, Ibaraki, Osaka, Japan
- MP 338 **Imaging Technologies for Constructing 3D Multimodal Lipid Atlases of the Eye;** David M. G. Anderson¹; Jeffrey D. Messenger²; Dongfeng Cao²; Nathan Heath Patterson³; Ankita Kotnala^{2, 3}; Lukasz G Migas⁴; Raf Van De Plas^{3, 4}; Richard M Caprioli³; Christine A. Curcio²; Kevin Schey³; Jeffrey M Spraggins³; ¹Vanderbilt University, Department of Biochemistry, Nashville, TN; ²University of Alabama at Birmingham, Birmingham, AL; ³Vanderbilt University, Nashville, TN; ⁴Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands
- MP 339 **Enhanced high-resolution spatially resolved lipidomics of multicellular tumor spheroids;** Fereshteh Zandkarimi¹; Rachel C. Avar¹; Laura J. Kaufman¹; ¹Department of Chemistry, Columbia University, New York, NY, 10027
- MP 340 **Chemical isotope labeling LC-MS metabolome analysis of small amounts of tissues procured by micro-punch for spatial metabolomics;** Michal Lazarek¹; Vi Tran¹; Liang Li^{1, 2}; ¹University of Alberta, Edmonton, AB; ²The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta
- MP 341 **MS3 imaging enables simultaneous mapping of phospholipid C=C and sn-position isomers;** Xiangyu Guo¹; Aojie Zhang²; Wenbo Cao¹; Qinhu Chen³; Wenpeng

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- Zhang¹; Zheng Ouyang¹; ¹State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; ²State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; ³Shenzhen Baoan Authentic TCM Therapy Hospital, Shenzhen, China
- MP 342 **Mass spectrometry imaging of single cells by tapping-mode scanning probe electrospray ionization;** Yoichi Otsuka^{1,2}; Kazuya Kabayama^{2,3}; Ayane Miura³; Koichi Fukase^{2,3}; Michisato Toyoda^{1,2}; ¹Department of Physics, Osaka University, Toyonaka, Japan; ²FRC, Osaka University, Toyonaka, Japan; ³Department of Chemistry, Osaka University, Toyonaka, Japan
- MP 343 **Mass spectrometry imaging of rigid biological sample;** Xin Diao^{1,2}; Jianing Wang^{1,2}; Zongwei Cai^{1,2}; ¹State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, Hong Kong SAR, China, Hong Kong, China; ²Department of Chemistry, Hong Kong Baptist University, Hong Kong, China
- MP 344 **Distribution analysis of galanthamine, a plant alkaloid, by MS imaging;** Kaoru Nakagawa¹; Tetsuo Iida¹; Satoshi Kasamatsu¹; Shuichi Shimma^{1,2}; Manami Kobayashi^{1,3}; ¹Shimadzu Corporation, Kyoto-city, Japan; ²Osaka University, Suita-city, Japan; ³Shimadzu Corporation, Kawasaki-city, Japan
- MP 345 **Sublimated/annealed aminated cinnamic acid analogs for high sensitivity 5µm MALDI IMS of lipids in human tissues;** Martin Dufresne¹; Angela Kruse¹; David M. G. Anderson¹; Lukasz G Migas²; Cody Marshall¹; Katerina V Djambazova¹; Nathan Heath Patterson¹; Raf Van De Plas²; Richard M Caprioli¹; Jeffrey M Spraggins¹; ¹Vanderbilt University, Nashville, TN; ²Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands
- MP 346 **Paint cross-section layer composition identification and prediction using MALDI-MSI;** Vaclav Krupicka¹; Florent Grelard¹; Landry Blanc¹; Julie Arslanoglu²; Nicolas Desbenoit¹; Caroline Tokarski¹; ¹Institute of Chemistry and Biology of Membrane and NanoObjects (CBMN), CNRS UMR 5248, Bordeaux Proteome, University of Bordeaux, Bordeaux, France; ²Department of Scientific Research, The Metropolitan Museum of Art, New York City, NY
- MP 347 **Improvement of Desorption Electrospray Ionization Mass Spectrometry Imaging for Oxysterols in the Atherosclerosis Mouse Model;** Cheng-Hung Yang¹; Mei-Ling Cheng¹; ¹Chang Gung University, Taoyuan, Taiwan
- MP 348 **Development of a single section MALDI-MSI-LC-MS/MS workflow for proteomics and quantitative lipidomics;** Tim Hendriks¹; Kasper K Krestensen¹; Giulia Sorbi²; Sara Tortorella²; Ron M.A. Heeren¹; Eva Cuypers¹; ¹Maastricht MultiModal Molecular Imaging Institute, Maastricht University, Maastricht, Netherlands; ²Molecular Horizon s.r.l, Bettona, Italy
- MP 349 **MS and MS2 Imaging for compound confirmation: MS, tMS2, ddMS2 approaches for AP-SMALDI-MS Imaging with Orbitrap MS;** Bernhard Spengler^{1,2}; Domenic Dreisbach³; Karl Christian Schäfer³; Carolin M Morawietz⁴; Kerstin Strupat⁵; ¹Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Gießen, Germany; ²TransMIT GmbH, Giessen, Germany; ³TransMIT GmbH, Giessen, Germany; ⁴Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Gießen, Germany; ⁵Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- MP 350 **FluoMALDI: a novel multimodal pipeline integrating fluorescence and MALDI imaging of a single sample through co-crystallization-enhanced fluorescence signals;** Xinyi Shen¹; Ethan Yang¹; Hoku West-Foyle¹; Dalton R Brown¹; Cole C Johnson¹; LaToya Roker¹; Caitlin M. Tressler¹; Ishan Barman²; Scot Kuo¹; Kristine Glunde¹; ¹Johns Hopkins University School of Medicine, Baltimore, MD; ²Johns Hopkins University, Baltimore, MD
- MP 351 **Advances in MALDI imaging of tryptic peptides: improved spatial resolution in mammalian tissue and first results for plant proteins;** Andreas Roempp¹; Bastian Jahreis¹; Oliver Wittek¹; ¹Bioanalytical Sciences and Food Analysis, University of Bayreuth, Bayreuth, Germany
- MP 352 **Systematic optimization of the DESI-MS imaging workflow to enhance detection of endogenous small molecule metabolites;** Meredith Spradlin^{1,2}; Livia S. Eberlin²; ¹The University of Texas at Austin, Austin, TX; ²Baylor College of Medicine, Houston, TX
- MP 353 **Measuring spatial resolution of different Mass Spectrometry Imaging modalities;** Martin Metodiev^{1,2}; Rory Thomas Steven³; Angeliki Christakopoulou³; Zoltan Takats^{2,4}; Josephine Bunch^{2,3,4}; ¹NPL, Teddington, United Kingdom; ²Imperial College, London, London, United Kingdom; ³National Physical Laboratory, Teddington, United Kingdom; ⁴Rosalind Franklin Institute, Harwell, Didcot, United Kingdom
- MP 354 **Spatiotemporal study of carbon metabolism in developing maize root tips with in vivo 13C labeling;** Pubudu Nuwan Perera Hapuarachchige¹; Young Jin Lee¹; ¹Iowa State University, Ames, IA
- MP 355 **Commercially ZnO NP matrix optimization for small molecule detection in rat brain by Matrix-Assisted Laser Desorption Ionization Mass Spectrometry Imaging;** Juan Pablo Galindo¹; Natalie Merola¹; Kristina Jurcic¹; Steven R. Laviolette¹; Ken K.-C. Yeung¹; ¹Western University, London, ON
- MP 356 **Novel reactive mass tags for the sensitive detection of steroidal ketones by MALDI MSI;** Rachel S. Pryce¹; Nassim Maarouf¹; Ayyoub Selka¹; Dominique Trudel¹; Fred Saad¹; Karina Gasbarrino²; Stella S. Daskalopoulou²; William D. Lubell¹; Pierre Chaurand¹; ¹University of Montreal, Montreal, QC; ²McGill University, Montreal, Québec
- MP 357 **Characteristics of a new caged matrix with high vacuum stability for MALDI mass spectrometry imaging;** Qiuqin Zhou¹; Stefano Rizzo²; Janina Oetjen³; Annabelle Fülöp¹; Miriam Rittner²; Hartmut Gilland²; Carsten Hopf^{1,4,5}; ¹CeMOS - Center for Mass Spectrometry and Optical Spectroscopy, Mannheim, Germany; ²Sirius Fine Chemicals SiChem GmbH, Bremen, Germany; ³Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ⁴Medical Faculty of Heidelberg University, Heidelberg, Germany; ⁵Mannheim Center for Translational Neuroscience (MCTN), Medical Faculty Mannheim, Heidelberg University, Mannheim, Germany
- MP 358 **Evaluation of a new poly-N-acetyllactosamine endo-β-galactosidase for multi-enzyme N-glycan MALDI imaging mass spectrometry tissue workflows;** Richard R Drake¹; Minyong Chen²; Grace Grimsley¹; Christopher H Taron²; ¹Medical University of South Carolina, Charleston, SC; ²New England Biolabs, Inc., Ipswich, MA
- MP 359 **Multi-Site Assessment of the MALDI HiPLEX-IHC Miralys System;** Kyle A Vanderschoot¹; Emily R. Sekera²; Gargey B. Yagnik³; Mark J. Lim³; Kenneth J. Rothschild³; Katherine A. Stumpo⁴; Amanda B. Hummon²; Erin H. Seeley⁵; Elizabeth K. Neumann⁶; ¹University of California, Davis, Davis, CA; ²The Ohio State University-Comprehensive Cancer Center, Columbus, OH; ³AmberGen, Inc., Billerica, MA; ⁴Bruker Scientific, LLC, Billerica, MA; ⁵University of Texas at Austin, Austin, TX; ⁶University of California Davis, Davis, CA
- MP 360 **Unsupervised co-registration of hematoxylin and eosin (H&E) stained microscopy images and mass spectrometry images (MSI) with feature filtering;** Sai Srikanth Lakkimsetty¹; Andreas Weber²; Kylie Ariel Bemis¹; Melanie Christine Föll²; Olga Vitek¹; ¹Northeastern University, Boston, MA; ²University of Freiburg, Freiburg, Germany
- MP 361 **Accurate Quantitative Mass Spectrometry Imaging via Aziridine-based Isobaric Tags Reveals Temporal and Spatial Changes of Isomeric Lipids in Medulloblastoma**

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- MP 363 **On-Tissue Derivatization for enhanced Carbohydrates and Sterols detection in Bombus Impatiens Bee via MALDI mass spectrometry; Nilay Saha¹; Andrew Goodenough¹; Taylor Hatcher¹; Michael Dillon¹; Franco Basile¹; ¹University of Wyoming, Laramie, WY**
- MP 364 **Optimization of embedding media for MALDI-mass spectrometry imaging of frozen tissue; Ching-Yuan Yang¹; Yatao Shi²; Yuan Liu²; Lingjun Li^{1,2}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI**
- MP 365 **Spatial single-cell multiomics using dual cluster ion beams secondary ion mass spectrometry (SIMS) imaging reveals 3D multilevel heterogeneities in liver; Hua Tian; University of Pittsburgh, Pittsburgh, PA**
- MP 366 **Unified and standardized mass spectrometry data processing in Python using spectrum_utils; Wout Bittremieux¹; Lev Levitsky²; Mateo Pilz³; Timo Sachsenberg³; Florian Huber⁴; Mingxun Wang⁵; Pieter C Dorrestein⁶; ¹University of Antwerp, Antwerpen, Belgium; ²Moscow institute of physics and technology, Moscow, Russia; ³University of Tübingen, Tübingen, Germany; ⁴Hochschule Düsseldorf, Düsseldorf, Germany; ⁵University of California Riverside, Riverside, CA; ⁶University of California San Diego, San Diego, CA**
- MP 367 **Improved identification of isomers using the High Dimensional Consensus Mass Spectral similarity algorithm; Deborah F McGlynn¹; Jason Eveleth^{1,2}; Nirina Rabe Andriamaharavo¹; Anthony Kearsley¹; ¹National Institute for Standards and Technology, Gaithersburg, MD; ²Brown University, Providence, RI**
- MP 368 **Novel DNN-powered quadrupole isolation profile analysis algorithm for improved speed, measurement robustness, and quality control; Adrian Schütz¹; Amelia Peterson¹; Bastian Reitemeier¹; Bernd Hagedorn¹; ¹Thermo Fisher Scientific, Bremen, Germany**
- MP 369 **High-throughput plasma proteomics to identify diabetes associated protein biomarkers and pQTLs; Harendra Guturu¹; Guhan Venkataraman¹; Amir Alavi¹; Ryan Benz¹; Khatereh Motamedchaboki¹; Anna Halama²; Frank Schmidt²; Karsten Suhre²; Serafim Batzoglou¹; ¹Seer, Inc., Redwood City, CA; ²Weill Cornell Medicine - Qatar, Education City, Qatar**
- MP 370 **Crema: an open-source Python tool for target-decoy false discovery rate estimation; Andy Lin¹; Donovan See²; Uri Keich³; William E Fondrie⁴; William Stafford Stafford²; ¹Pacific Northwest National Laboratory, Seattle, WA; ²University of Washington, Seattle, WA; ³University of Sydney, Sydney, Australia; ⁴Talus Bioscience, Seattle, WA**
- MP 371 **An automated computational pipeline for retention time alignment across LC systems; Ian Reah¹; Scott Trinkle²; Ryan P Marchand²; Chris Preston¹; Ian Morns¹; Richard Chapman²; Paul Fitch²; ¹Waters Corporation, Newcastle upon Tyne, United Kingdom; ²Waters Corporation, Milford, MA**
- MP 372 **Statistical analysis of tandem mass spectra; Felix Servant^{1,2}; Alexandre Giuliani^{1,2}; Laurent Nahon¹; ¹Synchrotron SOLEIL, L'Orme des Merisiers, Départementale 128, 91190 Saint-Aubin, France, Saint-Aubin, France; ²INRAE, UAR1008, Transform Department, Rue de la Géraudière, BP 71627,44316 Nantes, France, Nantes, France**
- MP 373 **Relative Probabilities of Library Search: A Comprehensive analysis of NIST/EPA/NIH EI and Tandem Libraries; Adva Baratz¹; Stephen E Stein²; ¹Israel Institute for Biological Research, Ness-Ziona, Israel; ²NIST, Gaithersburg, MD**
- MP 374 **Enhancing compound identification workflows with a novel library manager software application; Elizabeth Almasi¹; Emma E Rennie¹; James S Pyke¹; Tristan Chutka¹; Andrew McEachran¹; ¹Agilent Technologies, Santa Clara, CA**
- MP 375 **Sin.R: A SAINT-like AP-MS protein-interaction score implemented in R; Manor Askenazi¹; Beatrix Ueberheide²; Jackeline Ponce²; ¹Biomedical Hosting LLC, Arlington, MA; ²NYU Langone Health, New York, NY**
- MP 376 **MetaproDec: a new algorithm to appraise the quantitative composition of a microbiome based upon metaproteome; Jiahua Mu^{1,2}; Hongkai Xu^{1,2}; Yuxing Zhang²; Yamei Deng²; Da Qi²; Siqi Liu^{1,2}; ¹College of Life Sciences, University of Chinese Academy of Sciences, Beijing, China; ²Center of Proteomic Analysis, BGI Life Science Research Institute, Shenzhen, China**
- MP 377 **How well did you trap that ion? Find out with PeptidePrisoner!; Luis Mendoza¹; Michael R. Hoopmann²; Eric W. Deutsch²; Robert L. Moritz²; ¹Institute For Systems Biology, Seattle, WA; ²Institute for Systems Biology, Seattle, WA**
- MP 378 **SARS-CoV-2 Spike Protein Post Translational Modification Landscape and Its Impact on ProteinStructure and Functionvia Computational Prediction; Shaojun Tang; Hong Kong Center for Neurodegenerative Diseases, Hong Kong, China**
- MP 379 **Optimal transport-based LC-MS alignment algorithm; Stanislaw Jan Grodzki¹; Justyna Paulina Król¹; Michał Piotr Startek^{1,2}; Anna Barbara Gambin¹; ¹Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; ²Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany**
- MP 380 **Triqler for Data Independent Acquisition Data; Patrick Truong¹; Matthew The²; Lukas Kall¹; ¹Royal Institute of Technology, Stockholm, Sweden; ²Technical University of Munich, Freising, Germany**
- MP 381 **Estimating relative concentrations of analytes using computational optimal transport; Michał A. Ciach^{1,2}; Barbara Domżał¹; Michał Piotr Startek^{1,3}; Grzegorz Skoraczyński¹; Dirk Valkenburg²; Błażej Miasojedow¹; Anna Barbara Gambin¹; ¹Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; ²Hasselt University - DSI, Hasselt, Belgium; ³Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany**
- MP 382 **MassLite: An Integrated Python Platform for Single Cell Mass Spectrometry Data Pretreatment; Zhu Zou¹; Zhibo Yang¹; ¹Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK**
- MP 383 **Spectrum Averaging Algorithms for Increasing Mass Accuracy and Signal-to-Noise for Poorly Resolved and Low Abundance Peaks in Top-Down Proteomics; Nicholas E. Bollis¹; Austin V. Carr¹; Claire Boos¹; Lloyd M Smith¹; ¹University of Wisconsin-Madison, Department of Chemistry, Madison, WI**
- MP 384 **GlycoNetwork: A software for relating glycan expression with glycoenzyme activity; Xavier A Holmes¹; Michael Russelle S Alvarez¹; Armin Oloumi¹; Erin K. Morissette¹; Carlito B. Lebrilla¹; ¹University of California Davis, Davis, CA**
- MP 385 **Sensitivity analysis of isotope ratio measurements by MC-ICP-MS; Piotr Radziński¹; Jakub Karasiński¹; Andrii Tupys¹; Michał Piotr Startek^{1,2}; Anna Barbara Gambin¹; ¹University of Warsaw, Warsaw, Poland; ²iversity Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany**
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- Institute of Technology, Tokyo, Japan; ²China University of Geosciences, Wuhan, China; ³Tohoku University, Sendai, Japan
- MP 386 **ExclusionMS: A Software Tool for Customizable Precursor Selection in Tandem Mass Spectrometry;** Patrick T Garrett¹; Jeff Lane¹; Christopher Adams²; Tharan Sri Kumar²; Jonathan R Krieger²; Sven Brehmer²; John R. Yates III¹; ¹Scripps Research, La Jolla, CA; ²Bruker Daltonics GmbH & Co.KG, Bremen, Germany
- MP 387 **LC-MS MS1 image map classification enables real-time sample quality control for nanoparticle-based deep untargeted proteomics;** Biao Li¹; Ryan Benz¹; Harendra Guturu¹; Iman Mohtashemi¹; Theo Platt¹; Serafim Batzoglou¹; ¹Seer Inc., Redwood City, CA
- MP 388 **Real-time AI-Driven Data Acquisition for High-Throughput Proteomics;** Soroush Hajizadeh^{1,2,3}; Eric F Zaniewski¹; Benedikt C Clemens¹; Johannes Kreuzer^{1,2}; Dennis C. Sgroi^{1,2}; Daniel A. Haber^{1,2}; Lecia V. Sequest^{1,2}; Michael S. Lawrence^{1,2,3}; Wilhelm Haas^{1,2}; ¹MGH Cancer Center, Charlestown, MA; ²Harvard Medical School, Boston, MA; ³Broad Institute of MIT and Harvard, Cambridge, MA
- MP 389 **Gopher: Fast Gene Ontology Enrichment Analysis for Quantitative Proteomic Data;** Carolyn Allen¹; Lindsay K Pino¹; Sebastian Paez¹; William E Fondrie¹; ¹Talus Bioscience, Seattle, WA
- MP 390 **A novel cloud-native pipeline enabling deep, unbiased proteomics at extreme scale;** Seth Just¹; Andrew Nichols¹; Jian Wang¹; Iman Mohtashemi¹; Theodore Platt¹; Serafim Batzoglou¹; ¹Seer, Inc., Redwood City, CA
- MP 391 **Leveraging Python for Extending the Capability of MS Software Applications;** Stacey Simonoff¹; Yongdong Wang¹; Don Kuehl¹; ¹Cerno Bioscience, Las Vegas, NV
- MP 392 **Exact Formula for Positive False Discovery Rate (pFDR) Computation;** Justin Zhu¹; Henock Deberneh¹; Rovshan Sadygov¹; ¹UTMB at Galveston, Galveston, TX
- MP 393 **A complete solution for sequence variant analysis of recombinant antibodies and therapeutic proteins with electron-activated dissociation and automatic data processing;** Zhengwei Chen¹; Lei Xiong¹; ¹SCIEX, Redwood city, CA
- MP 394 **A GPU accelerated CDMS trap trajectory simulator and optimiser;** David Langridge¹; Keith Richardson¹; Jeff Brown¹; Kevin Giles¹; ¹Waters Corporation, Wilmslow, United Kingdom
- MP 395 **Enhanced performance for triple quadrupole mass spectrometry using in-line injection S-funnel interface;** Pearl Kwantwi-Barima¹; Isaac K. Attah¹; Reta Birhanu Kitata¹; Thomas L. Fillmore¹; Richard D. Smith¹; Yehia M. Ibrahim¹; Tujin Shi¹; ¹Pacific Northwest National Laboratory, Richland, WA
- MP 396 **Orbitrap Single Ion STORI Plots for Determination of Mean Free Path and Collision Cross Section;** Michael B Lanzillotti¹; James D Sanders²; Michael T Marty²; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX; ²The University of Arizona, Tucson, Arizona
- MP 397 **A preparative mass spectrometer to deposit native protein complexes on surfaces for high resolution imaging by cryoEM and SPM;** Paul Fremdling¹; Tim K Esser¹; Justin L P Benesch¹; Joseph Gault²; Stephan Rauschenbach¹; ¹University of Oxford, Dept. of Chemistry, Oxford, United Kingdom; ²Vertex Pharmaceuticals, Abingdon, United Kingdom
- MP 398 **A hybrid simulation-experimental approach for the design of mass spectrometer pumping system;** Tong Chen¹; Mark Werlich¹; John Nguyen¹; ¹Agilent Technologies, Santa Clara, CA
- MP 399 **Experimental Study of the Impact of Non-Linear Quadrupole Ion Guides on the Performance of a Triple Quadrupole Mass Spectrometer;** Matthias Lorenz¹; Anna Kornilova¹; Adrian MacLean¹; Tak Shun Cheung¹; Hamid Badiei¹; ¹PerkinElmer Inc., Woodbridge, ON
- MP 400 **Following Lasso Peptide Multistep Unthreading by LC-TIMS-UVPD-MS/MS;** Miguel Santos¹; Kevin Jeanne Dit Fouque¹; Julian Hegemann²; Francisco Fernandez-Lima¹; ¹Florida International University, Miami, FL; ²Technische Universität Berlin, Berlin, Germany
- MP 401 **Electrical Discharges - Fundamental Concepts and Mitigation Techniques for Maximising Detector Performance;** Aditya Wakhle¹; Antony N Jones¹; Russell J Jurek¹; David Whiteley¹; Kevin L Hunter¹; ¹IMI Adaptas, CLYDE, Australia
- MP 402 **Implementing a Concurrent Distributed Computing Architecture for Simulation of electrostatic Ion trap with Space Charge in Simion;** Ayla Osgood¹; Mark Osgood¹; Robert Jackson¹; ¹Ashwood Labs, Wilton, NH
- MP 403 **A phase-locked waveform generator for a rotating electric field mass analyzer;** Michael Espenship¹; Gregory Eakins¹; Julia Laskin¹; ¹Purdue University, WEST LAFAYETTE, IN
- MP 404 **BSA-mediated Henry Reaction in Microdroplets;** Mengyuan Xiao¹; Qi Wang¹; Richard N Zare²; Hao Chen¹; ¹New Jersey Institute of Technology, Newark, NJ; ²Stanford University, Stanford, CA
- MP 405 **MAXTOF, a novel program that determines optimal instrument parameters for MALDI-LTOF mass spectrometer;** Ko-Keng Chang^{1,2}; Yi-Hong Cai^{1,3}; Yi-Sheng Wang¹; ¹Genomics Research Center, Academia Sinica, Taiwan; ²Department of Chemistry, National Taiwan University, Taiwan; ³Department of Chemistry, National Taiwan Normal University, Taiwan
- MP 406 **Influence of Inlet Capillary Temperature on Charge Distributions of Submicrometer-sized Droplets and Particles with Electrospray Ionization;** Shao-Yu Liang¹; Li-Wei Hsieh¹; Huan-Cheng Chang²; Wen-Ping Peng¹; ¹National Dong Hwa University, Shoufeng, Hualien, Taiwan; ²Academia Sinica, Taipei, Taiwan
- MP 407 **A newly modified LAP-MALDI source coupled to a benchtop Q-TOF mass spectrometer and its effect on ion yields;** Selahaddin Sezgin¹; Ian Jones²; Jeff Brown³; Michael Morris³; Rainer Cramer¹; ¹Department of Chemistry, University of Reading, Reading, United Kingdom; ²Department of Biomedical Sciences, University of Reading, Reading, United Kingdom; ³Waters Corporation, Stamford Ave, Altrincham Road, Wilmslow, United Kingdom
- MP 408 **Modelling and observation of complex chemical noise patterns in high-resolution mass spectrometers;** Eugene Moskovets¹; Bogdan Budnik²; David H Perlman³; ¹MassTech Inc, Columbia, MD; ²Wyss Institute at Harvard, Boston, MA 02115; ³Merck & Co., Inc., Cambridge, MA
- MP 409 **Simulator for Eulerian and Lagrangian Ion Trajectories (SimELIT) and its Utility in Studying Ion Manipulations Across Pressure Scales;** Sandilya V.B. Garimella¹; Elizabeth H Denis¹; Cameron M. Giberson¹; Anjelica Bautusta¹; Rajesh K Singh¹; Gregory K Schenter¹; Jaehun Chun¹; Robert G. Ewing¹; ¹Pacific Northwest National Laboratory, Richland, WA
- MP 410 **Autonomous mass calibration of benchtop quadrupole Orbitrap™ mass spectrometers ensures continuous long-term operation and reliable drug compounds quantification;** Christian Klaas¹; Siegrun Mohring¹; Julia Kraegenbring¹; Catharina Crone¹; Claire Dauly¹; Alexander Harder¹; ¹Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- MP 411 **Use of High Resolution Ion Mobility (HRIM) for the Improvement of LC-MS/MS Data Quality;** Sergey Shulga-Morskoy¹; Suma Ramagiri²; Liulin Deng³; ¹Perkin Elmer Health Sciences Inc, Hopkinton, MA; ²PerkinElmer, Shelton, CT; ³MOBILion Systems, Inc, Chadds Ford, PA
- MP 412 **Machine learning physicochemical properties from DMS microsolvating environments explained by SHAP analysis;** Cailum MK Stienstra¹; Christian Ieritano¹; Alexander Haack¹; Scott Hopkins¹; ¹University of Waterloo, Waterloo, ON

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- MP 413 **Chemical Transformations can Occur during DMS Separations: Lessons Learned from Beer's Bittering Compounds**; Christian Ieritano¹; Alexander Haaack¹; Scott Hopkins¹; ¹University of Waterloo, Waterloo, ON
- MP 414 **Rapid Separation and Quantitation of $\Delta 8/\Delta 9$ -THC and other isobaric cannabinoids by Differential Mobility Spectrometry**; Christian Ieritano¹; Patrick Thomas¹; Scott Hopkins¹; ¹University of Waterloo, Waterloo, ON
- MP 415 **Exploring Isomer Separations and Structurally Specific Isotopic Shifts Using Next-Generation FAIMS Stages with Novel Buffers and Metal Cationization**; Hayden A Thurman¹; Pratima Pathak¹; Gordon A Anderson²; Alexandre A Shvartsburg¹; ¹Wichita State University, Wichita, KS; ²GAA Custom Electronics, LLC, Kennewick, Washington
- MP 416 **Orbitrap mass spectrometry and high-field asymmetric waveform ion mobility (FAIMS) enable in-depth, quantitative analysis of proteoforms <30 kDa**; Jake Kline¹; Michael W Belford²; Cornelia L Boeser²; Jingjing Huang²; David Bergen²; Kenneth R Durbin³; Joseph B Greer³; Graeme C McAlister²; Christopher Mullen²; Vlad Zabrouskov²; Luca Fornelli¹; ¹University of Oklahoma, Norman, OK; ²Thermo Scientific, San Jose, CA; ³Proteinacious, Evanston, IL
- MP 417 **Exploring protein N-glycosylation alterations between wild-type and mutant forms of Irisin**; Sayantani Chatterjee¹; Joshua A. Klein¹; Mu A^{3,4}; Quiyang Zhang³; Bruce M. Spiegelman^{3,4}; Joseph Zaia^{1,2}; ¹Department of Biochemistry, Center for Biomedical Mass Spectrometry, Boston University Chobanian & Avedisian School of Medicine, Boston, MA; ²Bioinformatics Program, Boston University, Boston, MA; ³Dana-Farber Cancer Institute, Boston, MA; ⁴Harvard Medical School, Boston, MA
- MP 418 **The development of new methods for formation, separation, detection, and identification of protomers using differential mobility spectrometry and mass spectrometry**; Andrew Finlay¹; Allyson G. Yee¹; Wojciech Gabryelski¹; W. Scott Hopkins²; ¹University of Guelph, Guelph, ON; ²University of Waterloo, Waterloo, ON
- MP 419 **Exploring FAIMS gas flow settings for optimal detection of post-translational modifications using LC-MS/MS**; Rosalie Chu¹; Chia-Feng Tsai¹; Karl K Weitz¹; Marina A Gritsenko¹; Ronald J Moore¹; Tao Liu¹; ¹Pacific Northwest National Laboratory, Richland, WA
- MP 420 **Improving Solvent Vapor Modification Through Ultrasonic Nebulization: Protic, Aromatic, and Nonclustering Solvent Systems for Isomeric Opioid Analysis with FAIMS-MS**; Nathan a Grimes¹; David Garbutt¹; Theresa Evans-Nguyen¹; ¹University of South Florida, Tampa, FL
- MP 421 **An Automated Workflow for the Quantification of 8-Different Antidepressants using LC-MS/MS**; Ramisa Fariha¹; Oluwanifemi D Okoh¹; Emma Rothkopf¹; Adam Spooner¹; Anubhav Tripathi¹; ¹Brown University, Providence, RI
- MP 422 **Challenges with the Bioanalysis of Phosphate Prodrugs and their Active Pharmaceutical Ingredients**; Kasie Fang¹; Timothy Sikorski¹; Zhuo Chen¹; Clara Andonian¹; Hermes Licea-Perez¹; ¹GSK, Collegeville, PA
- MP 423 **Fully automated and integrated 96-channel proteomics sample preparation platform applied for high-throughput drug target identification**; Ruijun Tian; Southern University of Science and Technology, Shenzhen, China
- MP 424 **Chemical derivatization combined with supercritical fluid chromatography to improve the resolution of stereoisomers**; Hermes Licea Perez; Bioanalysis / GSK, Collegeville, PA
- MP 425 **In-line Derivatization of Fatty Acids for LC-ESI-MS/MS Identification**; Anthony J Fanizza; Northern Illinois University (NIU), DeKalb, IL
- MP 426 **NRicher™: A Singular Low Abundance Proteome Enrichment Product Combines 6 Different Surface Features And Seamless Integration With On-Bead Digestion**; Matt Kuruc¹; Haiyan Zheng²; Amenah Soherwardy²; Swapan Roy¹; ¹Biotech Support Group LLC, Monmouth Junction, NJ; ²Rutgers University, New Brunswick, NJ
- MP 427 **Modular, scalable and automatable on-bead pipeline for bottom-up proteome and phosphoproteome profiling with built-in peptide and phosphopeptide fractionation**; Previn Naicker¹; Claire Koenig²; Ana Martinez Del Val²; Siphso Mamputha¹; Sindisiwe Buthelezi¹; Ireshyn S Govender^{1,3}; Isak Gerber^{1,3}; Justin Jordaan³; Stoyan Stoychev³; Jesper Velgaard Olsen²; ¹CSIR, Pretoria, South Africa; ²Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; ³ReSyn Biosciences, Pretoria, South Africa
- MP 428 **Miniaturization Strategies for Streamlined Drugs of Abuse Extraction prior to UHPLC-MS/MS Analysis**; Charlotte Hayes¹; Alan Edgington¹; Thomas Smith¹; Lee Williams¹; Adam Senior¹; Helen Lodder¹; Russell Parry¹; Lucy Lund¹; Zainab Khan¹; Geoff Davies¹; Claire Desbrow¹; Dan Menasco¹; ¹Biotage GB Limited, Cardiff, United Kingdom
- MP 429 **On-Column Digest Followed By SPE Desalting For Rapid And Simplified Sample Processing Without Sample Transfer**; Heather Eastwood¹; John D Laycock¹; Manuel Bauer²; Fabian Wendt²; Qi Huang¹; Shang Tsai¹; ¹Tecan, Baldwin Park, CA; ²Tecan, Männedorf, Switzerland
- MP 430 **Optimisation of sample preparation for the analysis of β -Methylamino-L-alanine in complex matrices**; Siobhan J Peters¹; Kenneth J Rogers¹; Simon M Mitrovic¹; David P Bishop¹; ¹UTS, Ultimo, Australia
- MP 431 **Determination of vedaprofen in livestock and fishery products using liquid chromatography-tandem mass spectrometry**; Bohyun Shin¹; Chohee Jeong¹; Sang Beom Han¹; ¹Department of Pharmaceutical Analysis, College of Pharmacy, Chung-Ang University, Seoul, South Korea
- MP 432 **Comparison between trypsin digestion and weak acid hydrolysis for characterization of various proteins using nanoLC-MS/MS**; Hyojin Hwang¹; Dokyung Kwon¹; Jeongkwon Kim¹; ¹Chungnam National University, Daejeon, South Korea
- MP 433 **Sample preparation-related technical variability of proteomic workflows incorporating multiplexed isobaric labeling and LC-MS/MS analysis**; Carly A. I. Twigg¹; Stefani N. Thomas¹; ¹Department of Laboratory Medicine and Pathology, University of Minnesota, Minneapolis, MN
- MP 434 **Bottom-Up Proteomic Workflows for Low Cell Input Samples in a Core Facility Setting**; Jennifer Roof¹; Hossein Fazelinia^{1,2}; Asif Amin Dar³; Hua C Ding¹; Lynn A Spruce¹; ¹CHOP-Penn Proteomics Core, Philadelphia, Pennsylvania; ²Department of Biomedical and Health Informatics, Children's Hospital of Philadelphia, Philadelphia, Pennsylvania; ³Children's hospital of Philadelphia, Philadelphia, Pennsylvania
- MP 435 **A novel two-cycle immunoaffinity enrichment strategy to enhance assay sensitivity of biotherapeutics in tissues**; Yipei Zhang¹; Mark G. Qian¹; Linlin Dong¹; ¹Takeda Development Center Americas, Cambridge, MA
- MP 436 **Identification of Low-Abundance Proteins in Biological Samples Using a Bottom-Up Approach on the ProTrap XG**; Victoria A Miller¹; Sara Lahsaee Little¹; Jessica L. Nickerson¹; Angela Giraldo²; Jean-François Noel²; Jean-Philippe Couture²; Hugo Gagnon²; ¹Allumiqs Corporation, Halifax, NS; ²PhenoSwitch Bioscience Inc., Sherbrooke, QC
- MP 437 **AutoPrep: fully automated, lossless proteomics sample preparation from lysate to protein concentration to contaminant-free, analysis-ready peptides - elute and shoot!**; John D Laycock¹; Heather Eastwood¹; Shang Tsai¹; Manuel Bauer²; Fabian Wendt²; John Wilson³; ¹Tecan, Baldwin Park, CA; ²Tecan, Männedorf, Switzerland; ³ProtiFi, LLC, Farmingdale, NY

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- MP 438 **Determination of atorvastatin calcium in human urine using LC-MS/MS;** Jie-ni Wang¹; He-Hsuan Hsiao¹; ¹Department of Chemistry, National Chung Hsing University, Taichung, Taiwan
- MP 439 **Normalizing MS Data: Extracted Lipids from Latent Fingerprints;** Aleesa E Chua¹; Leah Pfeifer¹; Heather Desaire¹; ¹University of Kansas, Lawrence, KS
- MP 440 **High-throughput method combining mass spectrometry and machine learning for analysis of fingerprint lipids for biomarker discovery;** Madeline Isom¹; Leah Pfeifer¹; Eden Go¹; Heather Desaire¹; ¹The University of Kansas, Lawrence, KS
- MP 441 **Lipidomic and Proteomic Plasma Evaluations Reveal Biomarkers for the Diagnosis of Domoic Acid Toxicosis in California Sea Lions;** Amie M. Solosky¹; Iliana M. Claudio²; Kaylie I. Kirkwood²; Rebecca L Beres¹; Michael G. Janech³; Frances M.D. Gulland⁴; Benjamin A. Neely⁵; Erin S. Baker⁶; ¹University of North Carolina Chapel Hill, Chapel Hill, NC; ²Department of Chemistry, North Carolina State University, Raleigh, NC; ³Department of Biology, College of Charleston, Charleston, SC; ⁴Wildlife Health Center, School of Veterinary Medicine, University of California, Davis, Davis, California; ⁵Chemical Sciences Division, National Institute of Standards and Technology, Charleston, SC; ⁶Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC
- MP 442 **Detailed kinetics measurements provide insights into competing fatty acyl chain loss from glycerophospholipid anions: why sn-2 loss is faster;** Samantha A Mehnert¹; Kimberly C Fabijanczuk¹; De'shovan M Shenault¹; Scott A McLuckey¹; ¹Purdue University, West Lafayette, IN
- MP 443 **Development of an offline 2D-LC lipidomics method;** Fernanda Monteiro Queiroz¹; Adriana Zardini Buzatto²; Liang Li^{1,2}; ¹University of Alberta, Edmonton, AB; ²The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta
- MP 444 **Development of automated MS/MS methods on an Orbitrap Fusion™ and a spectral database for in-depth lipidomic analysis of human plasma;** Vincent Marie¹; Benoit Colsch¹; François Fenaille¹; ¹Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), MetaboHUB, Gif sur Yvette, France
- MP 445 **An Efficient Monophasic Extraction Method for High-Throughput Bacterial Lipidomics;** Kingsley Bimpeh¹; Kelly M Hines¹; ¹University of Georgia, Athens, GA
- MP 446 **Establishing an LC-HRIM-MS workflow for targeted and untargeted lipidomic analyses;** Rachel Harris¹; Heidi Vitrac¹; Michelle English¹; James Atwood¹; ¹MOBILion Systems, Inc., Chadds Ford, PA
- MP 447 **Analysis of Lipids by Contained Electrospray Mass spectrometry with Online Fractionation using a Syringe-Based Solid Phase Extraction;** Octavion Spears¹; Benjamin J Burris²; Abraham Kwame Badu-Tawiah³; ¹the ohio state university, columbus, OH; ²agriculture and food, columbus, Ohio; ³The Ohio State University, Columbus, OH
- MP 448 **Electrospray ionization forms alkylated ammonium species that interfere with lipidomics analyses;** Joshua A Roberts¹; Aleksandra Bushueva¹; Meaghan Harley¹; Karl V Wasslen¹; Jeffrey C. Smith¹; ¹Carleton University, Ottawa, ON
- MP 449 **Functional role of ecdysteroids in awake and sleeping honey bee foragers;** Deepika Bais^{1,2}; Chhaya Patole²; Susanne Neupert¹; Axel Brockmann²; ¹University of Kassel, Kassel, Germany; ²National Centre for Biological Sciences, Bengaluru, India
- MP 450 **Investigation of in situ Lipids from EAE Mouse Brain Tissue using Mass Spectrometry Imaging;** Rawan Serena Kassim¹; Krista Berlin¹; Stephan B. Bach²; Thomas G. Forsthuber¹; ¹University of Texas at San Antonio, San Antonio, TX; ²University of Texas at San Antonio, San Antonio, TX
- MP 451 **Untargeted lipidomics of the Gemmata obscuriglobus bacterium under sterol synthesis inhibition conditions;** Franco Basile¹; Shelby Wakefield¹; Mitchell Helling¹; Seifeddine Ben Tekaya¹; Naomi Ward²; ¹University of Wyoming, Laramie, WY; ²Colorado State University, Fort Collins, CO
- MP 452 **Identification of Complex Triacylglycerols in Mouse Epididymal Adipose Tissue Using Ultra-performance Convergence Chromatography-Mass Spectrometry;** Yu-Ju Shih¹; Mei-Ling Cheng¹; ¹Chang Gung University, Taoyuan, Taiwan
- MP 453 **Fingerprinting the Unique Lipidome of Membrane Proteins Using Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry;** Jack P. Ryan¹; Yun Zhu²; Melanie T. Odenkirk³; Arthur Laganowsky²; Erin S. Baker¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC; ²Texas A&M University, College Station, TX; ³University of Arizona, Tucson, AZ
- MP 454 **Automation of lipid extraction with Hamilton Vantage system;** Weng Wong¹; James Joubert¹; Jay Leone¹; Peter Liu¹; Wendy Sandoval¹; Qingling Li¹; ¹Genentech, South San Francisco, CA
- MP 455 **Omega-6 Fatty Acid Oxidative Metabolism in Inflamed Dental Pulp;** Grace M Samenuk¹; Ken M Hargreaves¹; Qun Li¹; Stephan BH Bach²; Zakery James¹; ¹University of Texas Health San Antonio, San Antonio, TX; ²University of Texas San Antonio, San Antonio, TX
- MP 456 **Chemical and Physical Separation of Singly and Doubly Charged Lipids Within the Mass Spectrometer;** Kimberly Fabijanczuk¹; James W. Hager²; Scott A. McLuckey¹; ¹Purdue University, West Lafayette, IN; ²SCIEX, Concord, ON
- MP 457 **Using Lipid Exchange-Mass Spectrometry (LX-MS) to Uncover the Preferred Lipidome Environment Surrounding Membrane Proteins;** Melanie Odenkirk¹; Guozhi Zhang¹; Michael T Marty¹; ¹University of Arizona, Tucson, AZ
- MP 458 **Dual Metal Electrolysis Using a Theta Capillary for Lipid Analysis;** Annesha Sengupta¹; Madison Edwards¹; Xin Yan¹; ¹Department of Chemistry, Texas A&M University, College Station, TX
- MP 459 **4D Analysis of Lipid Nanoparticles (LNP) Component using Elute-timsTOF Pro 2 with VIP-HESI Source;** Beixi Wang¹; Xuejun Peng¹; Surendar Tadi²; Erica Forsberg¹; ¹Bruker Scientific, San Jose, CA; ²Bruker Scientific, Billerica, MA
- MP 460 **A discovery lipidomics workflow to maximize lipid identifications;** Vanessa Linke^{1,2,3}; Agnieszka Chacińska^{1,2}; Joshua J. Coon³; ¹Laboratory of Mitochondrial Biogenesis, IMol Polish Academy of Sciences, Warsaw, Poland; ²ReMedy International Research Agenda Unit, IMol Polish Academy of Sciences, Warsaw, Poland; ³Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- MP 461 **LIPID MAPS classifier: Machine learning approach for the prediction of the lipid class using the theoretical aggregated isotope distribution;** Annelies Agten¹; Heiko Neuweget²; Dirk Valkenborg¹; ¹Hasselt University - DSI, Hasselt, Belgium; ²Bruker Daltonik GmbH, Bremen, Germany
- MP 462 **Comparative lipidomic analysis of green algae Chlorella sorokiniana under nutritional stresses;** Hector Najera-Gonzalez¹; Claudio Cessar Barrera-Duarte¹; Luis R. Herrera-Estrella²; Damar Lopez-Arredondo¹; ¹Texas Tech University, Lubbock, Texas
- MP 463 **High Confidence Targeted Data Mining of Untargeted High-Resolution Data for Lipids;** Sheher Banu Mohsin¹; Mark Sartain²; Daniel Cuthbertson²; ¹Agilent Technologies, Wood Dale, IL; ²Agilent Technologies, Santa Clara, CA

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- MP 464 **Cellular Lipidomics with C=C Specificity Enabled by Aziridination**; Venus Pondevida¹; Jiaxin Feng¹; Xin Yan¹; ¹Texas A&M University, College Station, TX
- MP 465 **Aziridination-assisted mass spectrometry for nonpolar lipid analysis with isomer resolution**; Erin Hirtzel¹; Madison E Edwards¹; Dallas Freitas¹; Xin Yan¹; ¹Texas A&M University, College Station, TX
- MP 466 **Structural Characterization and Accurate Relative Quantitation of Unsaturated Lipid Isomers Enabled by Aziridination**; Xin Yan¹; Tingyuan Yang¹; Shuli Tang¹; ¹Texas A&M University, College Station, TX
- MP 467 **Pigment profiles in microalgae extracts by electron-transfer MALDI: the analyzer's influence**; Luis Miguel Díaz¹; Martha L Chacón-Patiño²; Chad R. Weisbrod²; Cristian Blanco-Tirado¹; Marianny Y. Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia; ²National High Magnetic Field Laboratory, Tallahassee, FL
- MP 468 **A quantitative discrimination study of recycled cashmere fibers using MALDI-TOF MS**; Shinya Koide¹; Yuzo Yamazaki²; Mizuki Ikoma¹; Aiko Yamaguchi¹; Shinichi Ohashi¹; ¹Quality Evaluation Institute, BOKEN, Osaka, Japan; ²Shimadzu Corporation, Kyoto, Japan
- MP 469 **Manufacture of 3D-printed portable spectrometer and MALDI-MS chips**; Yi-Ping Lee¹; Ting-Hsuan Wu¹; He-Hsuan Hsiao¹; ¹Department of Chemistry, National Chung Hsing University, Taichung, Taiwan
- MP 470 **Rationally Designed Synthetic Peptide as Versatile Calibrant to Improve the Accuracy of Protein Sequence Analysis using MALDI Mass Spectrometry**; Lingpeng Zhan¹; Yanyi Huang^{1,2}; Guanbo Wang^{1,2}; ¹Institute for Cell Analysis, Shenzhen Bay Laboratory, Shenzhen, China; ²Biomedical Pioneering Innovation Center, Peking University, Beijing, China
- MP 471 **Rapid Differentiation Between Mixed A1/A2 and A2 Only Cow Milk Using MALDI-TOF-MS**; Milaan Thirukumar¹; Francine E. Yanchik-Slade¹; Daniel Christensen²; Mohamed Boutaghou¹; ¹Shimadzu Scientific Instrument, Columbia, Maryland; ²Consolidated Lab Services, Knoxville, TN
- MP 472 **MALDI mass spectrometry enables rapid metabolic profiling of cerebrospinal fluid in Parkinson's disease**; Patrik Bjärterot¹; Theodosia Vallianatou¹; Anna Nilsson¹; Reza Shariatgorji¹; Per Svenningsson²; Per E Andren¹; ¹Uppsala University, Uppsala, Sweden; ²Karolinska Institutet, Stockholm, Sweden
- MP 473 **Integrated machine learning-based approach to evaluate authenticity in various food matrices via MALDI-TOF-MS technology**; Reza Aalizadeh¹; Anastasia S. Kritikou¹; Sofia K. Drakopoulou¹; Matthew Clabaugh²; Carsten Baessmann³; Nikolaos S. Thomaidis¹; ¹National and Kapodistrian University of Athens, Athens, Greece; ²Bruker Daltonics, Billerica, MA; ³Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- MP 474 **Advances in macromolecular materials research enabled by MALDI-TOF mass spectrometry**; Alyssa W May¹; Liam Reilly¹; Richard Reyes¹; Alex Claiborne¹; Marino Resendiz²; Megan Hill¹; Chris Ackerson¹; Eugene Y.-X. Chen¹; Travis S Bailey¹; ¹Colorado State University, Fort Collins, CO; ²University of Colorado, Denver, Denver, CO
- MP 475 **Imaging of Tissue pH by MALDI-TOF through In-Situ H/D Exchange**; Taylor A Murphree¹; Erik Cressman²; Miklos Guttman¹; ¹University of Washington, Seattle, WA; ²The University of Texas MD Anderson Cancer Center, Houston, TX
- MP 476 **Spatial Distribution of Pentacyclic Triterpenes in Cecropia spp roots using MALDI Imaging Mass Spectrometry**; Juan E. León-Jaimes¹; Luis M. Díaz-Sánchez¹; Guillermo Montoya²; Cristian Blanco-Tirado¹; Marianny Y. Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia; ²Universidad Icesi, Cali, Colombia
- MP 477 **Linking MALDI-FT-ICR phytoplankton pigment profiles with community taxonomy in a marine ecosystem**; Luis M. Díaz-Sánchez¹; Martha L. Chacón-Patiño²; Chad R. Weisbrod²; Julian Franco³; Janet Vivas³; Cristian Blanco-Tirado¹; Marianny Y. Combariza¹; ¹Universidad Industrial de Santander, Bucaramanga, Colombia; ²National High Magnetic Field Laboratory, Tallahassee, FL; ³Marine and Coastal Research Institute, Santa Marta, Colombia
- MP 478 **Novel MALDI-TOF screening workflow for rapid detection of host response to SARS-CoV-2**; Ryan Walsh¹; Greg Ourednik¹; Les Edinboro¹; ¹SpectraPass, Las Vegas, NV
- MP 479 **MALDI-MS for the analysis of cultural heritage materials**; Signe Vahur¹; Anu Teearu¹; ¹University of Tartu, Institute of Chemistry, Tartu, Estonia
- MP 480 **Improvements in Tissue Mimetic Models Using Gelatin Reinforcement and Sprayed Standards**; Andrew Bowman¹; Junhai Yang²; David S. Wagner²; ¹AbbVie, Inc., North Chicago, IL; ²AbbVie Inc., North Chicago, IL
- MP 481 **Investigating the performance of (liquid) AP-MALDI when fitted to a modified DESI source**; Jeff Brown¹; Emrys Jones¹; Michael Morris¹; Rainer Cramer²; ¹Waters Corporation, Wilmslow, United Kingdom; ²University of Reading, Reading, United Kingdom
- MP 482 **Development of a SALDI-MS approach for the specific and sensitive detection of biomolecules: focus on Alzheimer's disease biomarkers**; Aline Cournut¹; Paul Moustiez²; Yannick Coffinier²; Christine Enjalbal¹; Claudia Bich¹; ¹Univ. Montpellier, CNRS, ENSCM, IBMM, UMR5247, Montpellier, France; ²Univ. Lille, CNRS, UMR8520, IEMN, Lille, France
- MP 483 **Multi-laser induced MALDI post ionization (MALDI-2+) on a MALDI/ESI dual source**; Zhi Geng¹; Xiaoqiang Zhang¹; Wenjian Sun¹; ¹Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China
- MP 484 **Peptides Decorated C18-StageTip for the Detection of As3+ in Environmental Water with MALDI-MS**; Hua-Yun He¹; He-Hsuan Hsiao¹; ¹Department of Chemistry, National Chung Hsing University, Taichung, Taiwan
- MP 485 **Accurate mass calibration method for a target protein in the linear-mode of MALDI-TOF MS analysis**; Saeyoung Lee¹; Ju-Ri Park¹; Seohyun Hwang¹; Won Suk Yang¹; Je-Hyun Baek¹; ¹R&D Center for Clinical Mass Spectrometry, Seegene Medical Foundation, Seoul, South Korea
- MP 486 **Enhanced Performance of MALDI-TOF MS Analysis for Large Molecules by a Graphene-Coated Silicon Wafer Plate**; Yoon Kyung Choi¹; Dong Huey Cheon¹; Heejung Jang¹; Won Suk Yang¹; Je-Hyun Baek¹; ¹R&D Center for Clinical Mass Spectrometry, Seegene Medical Foundation, Seoul, South Korea
- MP 487 **Vapour deposition coated and recrystallised 9-aminoacridine method optimisation for MALDI MSI**; Hugo Delattre¹; Ariadna Gonzalez¹; Chelsea Nikula²; Lakshmi Nimishakavi¹; Daniel O'Connor¹; Melanie Bailey³; Josephine Bunch^{1,4}; Rory Steven¹; ¹National Physical Laboratory, Teddington, United Kingdom; ²Sanofi, Boston, MA; ³University of Surrey, Guildford, United Kingdom; ⁴Imperial College, London, London, United Kingdom
- MP 488 **Mobile ESI Sprayer Head for Matrix Application and On-Tissue Derivatization in MALDI-MSI**; Andrew E Paulson¹; Evan A Larson¹; Young Jin Lee¹; ¹Iowa State University, Ames, IA
- MP 489 **Optimization of small molecule MSI by delipidation, derivatization, and instrument tuning**; Lia Ficaro¹; Yik Siu¹; Mark Alu¹; Cynthia Loomis¹; Drew R. Jones¹; ¹NYU Langone Health, New York, NY
- MP 490 **Optimization of MALDI-MSI for spatial visualization of key metabolites in different sorghum root architectures**; Robert K. Stanley¹; Dusan Velickovic¹; Kevin J Zemaitis¹; Vimal Kumar Balasubramanian¹; Holly M. Andrews²; Laura K. Meredith²; Margot Bezruczyk³; Benjamin J. Cole³; Christopher R. Anderson¹; ¹Pacific

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- Northwest National Laboratory, Richland, WA; ²University of Arizona, Tuscon, Arizona; ³Lawrence Berkeley Laboratory, University of California, Berkeley, CA
- MP 491 **Automated well-to-well MALDI spotting and analysis using lower cost robotics and custom 3D-printed hardware;** Sadie R. Schultz¹; Garrett C. McFadden¹; Matthew M. Champion¹; ¹University of Notre Dame, Notre Dame, IN
- MP 492 **MALDI-TOF Mass Spectrometry: A tool for characterization of CBD Oils;** Les Edinboro¹; Greg Ourednik¹; Ryan Walsh¹; ¹SpectraPass, Las Vegas, NV
- MP 493 **Supraphysiological intravenous vitamin C administration promotes fatty acid β -oxidation and energy metabolism in humans;** Philenroza Thavrin¹; Jaewoo Choi¹; Ping Chen²; Qi Chen²; Jeanne Drisko²; Jan F. Stevens¹; ¹Oregon State University, Corvallis, OR; ²University of Kansas Medical Center, Kansas City, KS
- MP 494 **Doo Dots: An investigational platform for performing Dried Fecal Spot (DFS)-based bioanalysis;** Thomas D Horvath¹; Melinda A. Engevik²; Donald Chace³; ¹Texas Children's Hospital - Microbiome Center, Houston, TX; ²Medical University of South Carolina, Charleston, SC; ³Capitainer, Stockholm, Sweden
- MP 495 **A decision tree for diagnosing and phenotyping polycystic ovarian syndrome based on serum metabolic fingerprints;** Ruimin Wang¹; Lin Huang²; Kun Qian¹; ¹SJTU, Shanghai, China; ²Shanghai Chest Hospital, Shanghai, China
- MP 496 **Clinical MS in practice: bias removal and research results in the multicentre SAPHIRE statin metabolism clinical trial;** Eugene Goh¹; Lik Hang Wu²; Leroy S Pakkiri²; E Shyong Tai²; Jack Wei Chieh Tan²; Chester L. Drum²; ¹NUS, SINGAPORE, Singapore; ²National University of Singapore, Singapore, Singapore
- MP 497 **Metabolic Phenotypes Reflect Patient Sex and Injury Status: A Cross-Sectional Analysis;** Hope D Welhaven¹; Avery H Welfley¹; Prayag Pershad²; James Satalich²; Alexander C Vap²; Brian Bothner¹; Ron K June¹; ¹Montana State University, Bozeman, MT; ²Virginia Commonwealth University, Richmond, VA
- MP 498 **Quantitative analysis of Omega Fatty acids in human serum using Gas Chromatograph Mass Spectrometer;** Dr. Aseem Wagle¹; Prashant Hase¹; Bhaumik Trivedi¹; Sanket Chiplunkar¹; Durvesh Sawant¹; Rahul Dwivedi¹; Hemant Kesarkar¹; Dheeraj Handique¹; Dr. Pratap Rasam¹; Dr. Jitendra Kelkar¹; ¹Shimadzu Analytical India Pvt. Ltd., Mumbai, India
- MP 499 **Highly standardized metabolomic analysis of clinical samples using triple quadruple mass spectrometry;** Chandrashekhhar Honrao¹; Masoumeh Dorrani¹; Jifang Zhao¹; Chen Dong¹; Alessia Trimigno¹; Keri Sheehan¹; Elizabeth O'Day¹; Jurre Kamphorst¹; ¹Olaris Inc, Framingham, MA
- MP 500 **Five-hour bloodstream pathogen identification and antibiotic susceptibility testing using microbial metabolism directly from positive blood bottles with minimal sample preparation;** Thomas Rydzak¹; Ryan A Groves¹; Raied Aburashed¹; Maryam Mapar¹; Ian A Lewis¹; ¹University of Calgary, Calgary, AB
- MP 501 **Plasma Metabolomic Profiling for Diagnosis and Differentiation of Different Types of Cholestasis Diseases;** Juliana Magalhães De Oliveira^{1,2}; Martin Forbes²; Thais de Assis Lopes¹; Alex Aparecido Rossini Silva³; Juliana Goldbaum Crescente⁴; Michelle Hartz Braga⁴; Andréia de Melo Porcari³; Stefan Kempa²; Eduardo Luiz Rachid Cançado⁴; Regina Vincenzi Oliveira¹; ¹Federal University of São Carlos, São Carlos, Brazil; ²Max Delbrück Center for Molecular Medicine in the Helmholtz Association, Berlin Institute for Medical Systems Biology, Berlin, Germany; ³MS4Life Laboratory of Mass Spectrometry, Health Sciences Postgraduate Program, São Francisco University, Bragança Paulista, Brazil; ⁴Institute of Tropical Medicine, Department of Gastroenterology, Faculty of Medicine FMUSP, University of São Paulo, São Paulo, Brazil
- MP 502 **Multi-class assessment of chemical exposure in dried blood spots: a pilot study;** Vinicius Verri Hernandes^{1,2}; Maximilian Zeyda³; Lukas Wisgrill^{2,3}; Benedikt Warth^{1,2}; ¹Faculty of Chemistry, Department of Food Chemistry and Toxicology, University of Vienna, Währinger Straße 38, 1090, Austria; ²Exposome Austria, Research Infrastructure and National EIRENE Hub, Vienna, Austria; ³Department of Pediatrics and Adolescent Medicine, Comprehensive Center for Pediatrics, Medical University of Vienna, Austria
- MP 503 **Direct Probe Ionisation Mass Spectrometry applied to biomarker discovery in pancreatic cancer;** Neil Loftus¹; Alan Barnes¹; Emily G Armitage¹; Elon Correa²; Lynne Howells³; Sén Takeda⁴; Wen Chung⁵; ¹Shimadzu Corporation, Manchester, United Kingdom; ²Liverpool John Moores University, Liverpool, United Kingdom; ³Institute for Precision Health, The University of Leicester, Leicester, United Kingdom; ⁴Department of Anatomy, Teikyo University School of Medicine, Tokyo, Japan; ⁵Leicester HPB Unit, Glenfield Hospital, Leicester, United Kingdom
- MP 504 **LC-MS/MS Analysis of amino acid derived neurotransmitters and their metabolites in cerebrospinal fluid, and serum;** Rory M Doyle; WuXi Apptec- Research Services Division, Cranbury, NJ
- MP 505 **Development of a 96-well plate sample preparation method for multi-omics analysis using metabolomics and proteomics;** Kazuki Ikeda¹; Masatomo Takahashi²; Hata Kosuke²; Kohta Nakatani²; Shunsuke Aburaya²; Takeshi Bamba²; Yoshihiro Izumi²; ¹Kyushu University, Fukuoka, Japan; ²Medical Institute of Bioregulation, Fukuoka, Japan
- MP 506 **Evaluation of dried blood spot extraction strategies for untargeted metabolomics workflow;** Jiajun Lei¹; Cara L. Sake¹; John S. Chlystek¹; Jonathan E. Katz^{1,2}; ¹Lawrence J. Ellison Institute for Transformative Medicine, Los Angeles, CA; ²University of Southern California, Los Angeles, CA
- MP 507 **Evaluation of the Biocrates MxP Quant 500 kit on the Sciex 7500 QQQ LC-MS/MS for metabolomics analysis in liver;** Dan Su; WuXi Apptec- Research Services Division, San Diego, CA
- MP 508 **Development of Extraction Methods for Mitochondrial Membrane-Bound Products in Strain Engineering;** Ju Eun Jeon¹; Amy Lee¹; Peter Jackson¹; Nu Wang¹; Andrea Liu¹; Deborah Post¹; Michael Leavell¹; Mona Elbadawi¹; ¹Amyris, Emeryville, CA
- MP 509 **Evaluation of Red Blood Cell Depletion in Whole Blood Fractionation Workflows;** Sujatha Chilakala¹; Cara L. Sake¹; Ah Young Yoon¹; Jonathan E Katz^{1,2}; ¹Lawrence J. Ellison Institute for Transformative Medicine, Los Angeles, CA; ²USC, Los Angeles, CA
- MP 510 **Integration of MALDI-guided Laser Capture Microdissection to Enhance Spatial Metabolomics;** Jong Hee Song¹; Jessica K Lukowski¹; Minsoo Son¹; Antonia Zamacona Calderon¹; Byoung-Kyu Cho¹; Young Ah Goo¹; ¹Mass Spectrometry Technology Access Center at the McDonnell Genome Institute at Washington University School of Medicine, St. Louis, MO
- MP 511 **Optimizing protocols to profile metabolites and lipids from individual organs of adult zebrafish;** Darshak Gadara¹; Michaela Schwaiger-Haber¹; Madelyn M. Jackstadt¹; Madison Barr¹; Leah P. Shriver¹; Gary J. Patti¹; ¹Washington University in St. Louis, St. Louis, MO
- MP 512 **Adopting Orphan Metabolites of Microbiota: MS-based Biochemical and Metagenomic Characterization;** Sungwhan F Oh; Brigham and Women's Hospital, Boston, MA
- MP 513 **A high-throughput microflow DIA workflow for bacterial proteomics;** Miriam Abele¹; Etienne Doll²; Florian P. Bayer³; Chen Meng¹; Klaus Neuhaus⁴; Siegfried Scherer²; Bernhard Kuster^{1,3}; Christina Ludwig¹; ¹BayBioMS, TUM, Freising, Germany; ²Research Department Molecular Life Sciences, TUM, Freising, Germany; ³Chair of Proteomics

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- and Bioanalytics, TUM, Freising, Germany; ⁴Core Facility Microbiome, ZIEL – Institute for Food & Health, TUM, Freising, Germany
- MP 514 **Investigating Squid-Vibrio symbiosis using MALDI-tims-qTOF-IMS**; Allyson McAtamney¹; Denise A Ludvik²; Shaimaa M Aboukhatwa^{3,4}; Laura M Sanchez¹; Mark J Mandel²; Terry W Moore³; ¹Department of Chemistry and Biochemistry, University of California, Santa Cruz, Santa Cruz, California; ²Department of Medical Microbiology and Immunology, University of Wisconsin-Madison, Madison, WI; ³Department of Pharmaceutical Sciences, University of Illinois at Chicago, Chicago, IL; ⁴Department of Pharmaceutical Chemistry, Tanta University, Tanta, Egypt
- MP 515 **Metaproteomics with advanced phylogenetic search space filtering in MaxQuant**; Jinqiu Xiao¹; Shamil Urazbakhitin¹; Juergen Cox¹; ¹Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Martinsried, Germany
- MP 516 **The metabolic landscape of infant gut microbiome revealed by MS-Metabolomics in a gut simulator**; Shiqi Zhang¹; Li Chen¹; Ming Hu¹; Jiangjiang Zhu^{1,2}; ¹The Ohio State University, Columbus, OH; ²The Ohio State University-Comprehensive Cancer Center, Columbus, OH
- MP 517 **Metaproteomics characterization of Svalbard permafrost active layer reveals post-thaw metabolic activities and adaptations of subsurface microbes to a warming environment**; Samantha Peters¹; Richard J Giannone¹; Katie Sipes²; Fumnyanya Abua²; Renxing Liang³; Andrey Abramov⁴; Julia Boike^{5,6}; Tatiana Vishnivetskaya²; Karen Lloyd²; Robert L Hettich¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Tennessee, Knoxville, TN; ³Princeton University, Princeton, NJ; ⁴Institute of Physicochemical and Biological Problems in Soil Science, Pushchino, Russia; ⁵Alfred Wegener Institute Helmholtz-Center for Polar and Marine Research, Potsdam, Germany; ⁶Humboldt-Universität zu Berlin, Berlin, Germany
- MP 518 **The role of microbial siderophores in the central nervous system and pulmonary infections**; Dominika Luptáková¹; Rutuja Hiraji Patil¹; Miloš Petřík²; Jan Hrbáček³; Hynek Mácha¹; Andrea Palyzová¹; Tereza Juříková¹; Radim Dobiáš⁴; David Alec Stevens^{5,6}; Vladimír Havlicek¹; ¹Institute of Microbiology of the Czech Academy of Sciences, Prague 4, Czech Republic; ²Institute of Molecular and Translational Medicine, Olomouc, Czech Republic; ³Faculty Thomayer Hospital, Prague 4, Czech Republic; ⁴Public Health Institute, Ostrava, Czech Republic; ⁵California Institute for Medical Research, San Jose, CA; ⁶Stanford University School of Medicine, Stanford, Czech Republic
- MP 519 **Automated bacterial sample preparation from Agar to MALDI target for routine bacterial identification**; Michael Douglas Nairn¹; Philip Kirk²; Matthew Openshaw¹; Oliver Severn²; Leah Ashley²; ¹Shimadzu, Manchester, UK, Manchester, United Kingdom; ²Singer Instruments, Roadwater, United Kingdom
- MP 520 **Comparison of Protein Extraction Methods and Data Analysis Strategies for Metaproteomic Soil Analysis**; Abigale S Mikolitis¹; Ethan McBride¹; Marie Kroeger¹; Trevor Glaros¹; Philip Mach¹; ¹Los Alamos National Laboratory, Los Alamos, NM
- MP 521 **Mass spectrometry-guided precision medicine: a new frontier for clinical microbiology**; Ian Lewis¹; Daniel B. Gregson^{1,2}; Fiona Clement¹; Ashlee Earl³; Yonatan Grad⁴; Hallgrímur Benediktsson^{1,2}; Bruce Walker³; M. Ethan McDonald¹; ¹University of Calgary, Calgary, AB; ²Alberta Precision Laboratories, Calgary, AB, Canada, Calgary, AB; ³Broad Institute of MIT and Harvard, Cambridge, MA; ⁴Harvard T.H. Chan School of Public Health, Boston, MA
- MP 522 **Assessing the effects of exogenous fatty acids and FASII inhibitors on lipid profiles and daptomycin susceptibilities of Staphylococcus aureus**; Keerthi Appala¹; Kelly M Hines¹; ¹University of Georgia, Athens, GA
- MP 523 **Pseudomonas aeruginosa - Rhizopus microsporus interaction: a metabolomics hunt for an antifungal treatment for Mucormycosis**; Emily C. Giedraitis¹; Vanessa V. Phelan¹; ¹Department of Pharmaceutical Sciences, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of Colorado, Anschutz Medical Campus, Aurora, CO
- MP 524 **A Targeted and Rapidly Expandable LC-MS/MS Platform for Deciphering the Relationship between SCFAs, Fiber, and the Gut Microbiome**; Cheng-Yu Charlie Weng¹; Christopher Suarez¹; Karen Kalanetra¹; Chad Masarweh¹; David A. Mills¹; Carlito B. Lebrilla¹; ¹UC Davis, Davis, CA
- MP 525 **Simplified molecular imaging analysis of excreted microbial metabolites using a benchtop MALDI-TOF system**; Sidrah Rahman¹; Michael Douglas Nairn²; Rian Griffiths³; Tom K. Abban⁴; ¹School of Pharmacy, University of Nottingham, Nottingham, United Kingdom; ²Shimadzu, Manchester, UK, Manchester, United Kingdom; ³School of Pharmacy, University of Nottingham, Nottingham, United Kingdom; ⁴Shimadzu, Manchester, UK, Manchester, United Kingdom
- MP 526 **Spent media analysis and metabolic modelling of recombinant E. coli**; Pramod P Wangikar^{1,2}; Hardik Dodia¹; Vivek Mishra²; Bhushan Burkul²; Charandatta Muddana²; Anant Kedia²; Prajval Nakrani²; Sneha Rana³; ¹Indian Institute of Technology Bombay, Mumbai, India; ²Clarity Bio Systems India Pvt Ltd, Pune, India; ³Indian Institute of Technology, Bombay, Mumbai, India
- MP 527 **Spent amino acid analysis opens paths to improve recombinant protein production in complex media**; Hardik Dodia¹; Vivek Mishra^{2,3}; Deepti S¹; Pramod P Wangikar^{1,3}; ¹Indian Institute of Technology Bombay, Mumbai, India; ²Indian Institute of Technology, Bombay, Mumbai, India; ³Clarity Bio Systems India Pvt Ltd, Pune, India
- MP 528 **Method comparison of innovative bioinformatics tools for a rapid visualization of sample-specific signals of bacterial co-culture by mass spectrometry imaging**; Pierre Burguet¹; Raphaël La Rocca¹; Christopher Kune¹; Alexandre Bastin¹; Déborah Tellatin¹; Sébastien Rigali¹; Loïc Quinton²; ¹University of Liege, Liege, Belgium; ²University of Liège, Liège, Belgium
- MP 529 **Probability-based taxonomic profiling of microbiome samples using PepGM and Unipept**; Tanja Holstein^{1,2,3}; Pieter Verschaffel^{2,4}; Lennart Martens^{2,3}; Thilo Muth⁵; ¹Bundesanstalt für Materialforschung - und Prüfung, Berlin, Germany; ²VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; ³Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; ⁴Department of Applied Mathematics, Computer Science, and Statistics, Ghent University, Ghent, Belgium; ⁵Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany
- MP 530 **Multiple targeted methods to elucidate dynamic changes to microbially-derived metabolites following xanthohumol supplementation in healthy adults**; Paige E. Jamieson¹; Eli Smart¹; Gabriella Brown¹; Jaewoo Choi¹; Ryan Bradley²; Thomas O. Metz³; Jan Frederik Stevens¹; ¹Oregon State University, Corvallis, OR; ²National University of Natural Medicine, Portland, Oregon; ³PNNL, Richland, WA
- MP 531 **Using RTMS to Unravel the Microbiome Molecular Mechanisms of Carbon and Nutrient Cycling during Rewetting after Drought**; Mary S Lipton¹; Karl K Weitz¹; Montana L Smith¹; James J Moran²; ¹Pacific Northwest National Laboratory, Richland, WA; ²Michigan State University, East Lansing, MI
- MP 532 **Changes in the gut metaproteome of women with different body mass index status**; Gustavo Diaz¹; Kitty Brown¹; Amirmansoor Hakim²; Corey Broeckling¹; Jessica Prenni³; Mikayla A. Borton⁴; Kelly C. Wrighton⁴; ¹Analytical Resources Core: Bioanalysis and Omics, Colorado State University, Fort Collins, CO; ²ThermoFisher Scientific, San

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- Jose, CA; ³Department of Horticulture and Landscape Architecture, Colorado State University, Fort Collins, CO; ⁴Department of Soil and Crop Science, Colorado State University, Fort Collins, CO
- MP 533 **Proteome-wide size exclusion ICPMS analysis of native metalloprotein complexes in bacteria and archaea;** James D Larson¹; Monika Tokmina-Lukaszewska¹; Hunter Fausset¹; Gwendolyn Cooper¹; Scott Spurzem¹; Savannah Cox¹; Rachel Spietz¹; Brooklynn Brekke¹; Jordan Pauley¹; Eric Boyd¹; Brian Bothner¹; ¹Montana State University, Bozeman, MT
- MP 534 **Targeted Metabolomics to unveil gut metabolite signatures identifies quinic acid as disease promoting factor in endometriosis;** Chandni Talwar¹; Pooja Popli¹; Satwikreddy Putluri²; Chandrasekhar R. Ambati²; Abu Hena Mostafa Kamal²; Ramakrishna Kommagani¹; ¹Department of Pathology and Immunology, Baylor College of Medicine, One Baylor Plaza, Houston, TEXAS; ²Department of Molecular and Cellular Biology, Baylor College of Medicine, One Baylor Plaza, Houston, TEXAS
- MP 535 **The postmenopausal urinary metabolome is associated with recurrent UTI and urobiome ecology;** Michael L. Neugent¹; Neha V. Hulyalkar¹; Philippe E. Zimmern²; Vladimir Shulaev³; Nicole J. De Nisco^{1,2}; ¹Department of Biological Sciences, The University of Texas at Dallas, Richardson, Texas; ²Department of Urology, The University of Texas Southwestern Medical Center, Dallas, Texas; ³Department of Biological Sciences, The University of North Texas, Denton, Texas
- MP 536 **Accounting for chimeric spectra boosts the number of identifications in metaproteomics without impacting sensitivity;** Tim Van Den Bossche^{1,2}; Lennart Martens^{1,2}; Viktoria Dorfer³; ¹VIB - UGent Center for Medical Biotechnology, Gent, Belgium; ²Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; ³Bioinformatics Research Group, University of Applied Sciences Upper Austria, Hagenberg, Austria
- MP 537 **Data-Independent Acquisition Mass Spectrometry as a Tool for Metaproteomics: Cross-Laboratory Methodological Comparisons Using a Model Microbiome;** Andrew T. Rajczewski¹; Jose Alfredo Blakeley-Ruiz²; Matthew R. McIlvin³; Annaliese Meyer³; Tim Van Den Bossche⁴; Brian C Searle⁵; Timothy J Griffin¹; Makoto Saito³; Manuel Kleiner²; Pratik D Jagtap¹; ¹University of Minnesota, Minneapolis, MN; ²North Carolina State University, Raleigh, NC; ³Woods Hole Oceanographic Institution, Falmouth, MA; ⁴Ghent University, Ghent, Belgium; ⁵Ohio State University, Columbus, OH
- MP 538 **LC-MS Analysis of the Effects of Oral Contraceptives on the Human Gut Microbiome;** Danielle A Beefas¹; Myedith R Damba¹; Ellen Kuang¹; Christopher R Harrison¹; ¹San Diego State University, San Diego, CA
- MP 539 **Discovery and identification of a non-lethal mechanism for intercolony inhibition ("sibling rivalry") in *Marinobacter*;** Ellen Kuang¹; Heather Thorogood¹; Mary W Carrano¹; Erica M Forsberg^{1,2}; Carl J Carrano¹; ¹San Diego State University, San Diego, CA; ²Bruker Scientific, LLC, Billerica, MA
- MP 540 **Nextgen Metaproteomics: Metaproteomics analysis using predicted deep learning library searching;** Pratik Dilip Jagtap¹; Subina P Mehta¹; Wassim Gabriel²; Andrew T. Rajczewski¹; James Johnson¹; Reid Wagner¹; Mathias Wilhelm²; Brian C Searle³; Timothy J Griffin¹; ¹University of Minnesota, Minneapolis, MN; ²Computational Mass Spectrometry, Technical University of Munich, Freising, Germany; ³The Ohio State University, Columbus, OH
- MP 541 **Temporal profiling of the extracellular proteome secreted by *Escherichia coli* during biofilm formation on various mannose surfaces;** Mengfan Wang¹; Guoting Qin¹; Chengzhi Cai¹; Jennifer Copeland²; Huamin Cai²; ¹University of Houston, Houston, TX; ²VICI Valco Instrument, Houston, TX
- MP 542 **Temporal profiling of the extracellular proteome secreted by *Escherichia coli* 83972 during biofilm formation on catheters pretreated with human urine;** Rufeng Li¹; Guoting Qin¹; Mengfan Wang¹; Jennifer Copeland²; Huamin Cai²; Chengzhi Cai¹; ¹University of Houston, Houston, TX; ²VICI Valco Instruments, Houston, TX
- MP 543 **Microbiota-Dependent Metabolomic Changes Nutritional Intervention during Pregnancy;** Emma R Guiberson¹; Brian Defelice²; Josh Elias²; Justin L Sonnenburg^{1,2,3}; ¹Department of Microbiology and Immunology, Stanford University, Palo Alto, CA; ²Chan-Zuckerberg Biohub, San Francisco, CA; ³Center for Human Microbiome Studies, Stanford University, Palo Alto, CA
- MP 544 **Thread-Based Microfluidic Device for Real-Time Reaction Monitoring by Thread Spray Mass Spectrometry;** Salmika G Wairegi¹; Abraham Kwame Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- MP 545 **Photoswitch-decorated nanoparticle for on-chip protein separation and mass spectrometric determination;** Tanushree Dutta¹; Julea Vlassakis¹; ¹Rice University, Houston, TX
- MP 546 **High-Throughput Ultra-Low Flow LCMS platform for low sample amount proteome profiling;** Paul Jacobs¹; Santosh Renuse²; Xuefei Sun³; Yuan Lin³; Jeff Op De Beeck¹; ¹Thermo Fisher Scientific - Belgium, Ghent, Belgium; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, Sunnyvale, CA
- MP 547 **Use of microchip capillary electrophoresis – mass spectrometry for automated rapid measurement of enzyme reaction kinetics;** Gili Ben-Nissan¹; David Morgenstern¹; Simon Krabbe²; J. Will Thompson²; Scott Mellors²; Yishai Levin¹; Michal Sharon¹; ¹Weizmann Institute of Science, Rehovot, Israel; ²908 Devices, Inc., Boston, MA
- MP 548 **Combining capillary electrophoresis and trapped ion mobility spectrometry mass spectrometry to analyze epitranscriptomic marks mediating virus-host interactions in infectious diseases;** Daniele Rollo¹; Adi M Kulkarni²; Kate Yu²; Guillaume Tremintin³; Daniele Fabris¹; ¹University of Connecticut, Storrs, CT; ²908 Devices, Inc., Boston, MA; ³Bruker Daltonics, San Jose, CA
- MP 549 **A Novel Sensitive Top-down RPLC-CE-MS System for the Analysis of Sub-microgram Intact Cell Lysate;** Samin Anjum¹; Yanting Guo¹; Zhitao Zhao¹; Kellye A Cupp-Sutton¹; Si Wu¹; ¹University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK
- MP 550 **Exploring the possibilities for Microchip SPE-CE-MS;** J. Scott Mellors¹; J. Will Thompson¹; Erin A. Redman¹; ¹908 Devices, Inc., Carrboro, NC
- MP 551 **Microfluidics: Streamlining ink identification using mass spectrometry;** Morgan Demmler¹; Nelson R Vinuesa^{1,2}; ¹Wilson College of Textiles, NC State University, Raleigh, NC; ²Department of Chemistry, NC State University, Raleigh, NC
- MP 552 **Mass spectrometry of model primordial peptides for origins and astrobiology research;** Jay G Forsythe; College of Charleston, Charleston, SC
- MP 554 **MAPPs (MHC-I/II-Associated Peptide ProteomicS) revolutions: an evolute in vitro tool to assess immunogenicity risks;** Axel Ducret¹; Maureen Bardet¹; Katharina Hartman¹; Rebecca Xicluna¹; Céline Marban-Doran¹; ¹Roche Innovation Center Basel, Basel, Switzerland
- MP 555 **Evaluation of Multifarious MHC Class II Antibodies for Use as Immunoaffinity Enrichment Reagents in MHC Associated Peptide Proteomics (MAPPs);** Jason Lamar¹; M. Violet Lee¹; Sylvia C Wong¹; Peter Tran¹; Ola Saad¹; ¹Genentech Inc., South San Francisco, CA
- MP 556 **Spatial Neuropeptide Analysis of Small Neuronal Ganglia in Blue Crab *Callinectes sapidus* Informed by Multimodal Mass Spectrometry;** Thao Duong¹; Ashley Phetsanthad¹; Peng-Hsuan Huang¹; Vu Ngoc Huong Tran²;

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- MP 557 **Circadian neuropeptidomics for the analysis of coupling factors controlling multiscale behavioral rhythms in *Drosophila melanogaster***; Susanne Neupert¹; Deepika Bais¹; Anna-Sophie Kuegler¹; Anna C Schneider¹; ¹University of Kassel, Kassel, Germany
- MP 558 **Improving Mass Spectrometry-Based Detection and Identification of Neuropeptides in Crustacean Hemolymph Using an Anticoagulant Buffer**; Angel E. Ibarra¹; Wenxin Wu¹; Lingjun Li^{1,2}; ¹University of Wisconsin-Madison, Department of Chemistry, Madison, WI; ²University of Wisconsin-Madison School of Pharmacy - Madison, WI, Madison, WI
- MP 559 **Workflow for rapid automated immunopeptidome profiling**; Stoyan Stoychev¹; Justin Jordaan²; Terry Lim³; Pouya Faridi³; ¹ReSyn BioSciences, Pretoria, South Africa; ²ReSyn Biosciences, Pretoria, South Africa; ³Monash University, Melbourne, Australia
- MP 560 **Time-of-Day Analysis of the CSF Peptidome by nanoLC-QqTOF**; Shannon D Berneche¹; Taylor Jorgensen¹; Wei-Chun Kao¹; Dharmesh Parmar²; Martha Gillette^{1,3}; Jonathan V. Sweedler^{1,2}; ¹Neuroscience Program, University of Illinois at Urbana-Champaign, Urbana, IL; ²Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana and Champaign, IL; ³Department of Cell and Developmental Biology, University of Illinois at Urbana-Champaign, Urbana, IL
- MP 561 **Immunopeptidomic profiling from soluble HLA in human plasma by ultra-high sensitive mass spectrometry**; Maria Wahle¹; Maximilian Zwiebel¹; Wen-Feng Zeng¹; Patricia Skowronek¹; Marvin Thielert¹; Matthias Mann^{1,2}; ¹Max-Planck-Institute for Biochemistry, Martinsried, Germany; ²Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark
- MP 562 **An optimized biochemical and analytical workflow to unravel the human plasma peptidome**; Andreas Zellner¹; Steffen Tiedt²; Chien-Yun Lee¹; ¹Young Investigator Group: Mass Spectrometry in Systems Neurosciences, School of Life Sciences, Technical University of Munich, Munich, Germany; ²Institute for Stroke and Dementia Research, University Hospital, LMU Munich, Germany, Germany
- MP 563 **High sensitivity HLA-I and HLA-II immunopeptidomics on the TIMS-TOF Pro-2 Mass Spectrometer with Thunder-DDA-PASEF and HLA-tailored DIA-PASEF**; David Gomez-Zepeda^{1,2}; Annica Preikschat^{1,2}; Julian Beyrle^{1,2}; Stefan Tenzer^{1,2}; ¹HI-TRON, Deutsches Krebsforschungszentrum (DKFZ), Mainz, Germany; ²Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany
- MP 564 **A novel deep learning-based workflow for analysing immunopeptidome data generated by Data Independent Acquisition (DIA)**; Qing Zhang¹; Kyle Hoffman¹; Sahar Rabinoviz¹; Chao Peng²; Lei Xin¹; Baozhen Shan¹; ¹Bioinformatics Solutions Inc, Waterloo, ON; ²BaizhenBio Inc., shanghai, China
- MP 565 **Sensitive, high-throughput single-shot HLA-I and HLA-II immunopeptidomics with improved coverage using data dependent parallel accumulation-serial fragmentation mass spectrometry**; Kshiti Meera Phulphagar¹; Claudia Ctortekca¹; Alvaro Sebastian Vaca Jacome²; Susan Klaeger³; Eva Verzani¹; Gabrielle Hernandez¹; Karl R Clauser¹; Jennifer G Abelin¹; Steven A Carr¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²Bruker Daltonics, San Jose, CA; ³Genentech Inc, South San Francisco, CA
- MP 566 **Neuropeptidome Profiling of the Ascaris suum Body Cavity Fluid**; Wenxin Wu¹; Ciaran McCoy²; Darrin McKenzie²; Louise Atkinson²; Angela Mousley²; Lingjun Li¹; ¹University of Wisconsin Madison, Madison, WI; ²Queen's University Belfast, Belfast, United Kingdom
- MP 567 **Enhancing the detection of MHC I-bound peptides on the TimsTOF Pro**; Daniel Flender^{1,2}; Geert Baggerman^{1,2}; Kurt Boonen^{1,2}; Elise Pepermans¹; ¹University of Antwerp, Antwerpen, Belgium; ²VITO - Flemish Institute for Technological Research, Mol, Belgium
- MP 568 **Investigation of the immunopeptidome from multiple genetically different major histocompatibility (MHC) alleles by mild acid elution (MAE) for vaccine development**; Teesha C Baker¹; Lucy Song¹; Charley Cai¹; Selwyn Gu¹; Leonard J. Foster¹; ¹University of British Columbia, Vancouver, BC
- MP 569 **Algorithm-assisted peptidomic diagnosis of clinical mycobacteria isolates**; Jia Fan¹; Sudipa Maity¹; Duran Bao¹; Bo Ning¹; Adrian Zelazny²; Tony Hu¹; ¹Tulane University School of Medicine, New Orleans, LA; ²NIH/Clinical Center, Bethesda, MD
- MP 570 **Understanding Phosphotyrosine Signaling at the Single Spheroid Level**; Brian D Fries¹; Alissa Nelson²; Amanda B Hummon¹; ¹The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; ²Cell Signaling Technology, Danvers, MA
- MP 571 **Assessing insulin signaling responses by protein phosphorylation surveillance in plasma extracellular vesicles**; Yi-Kai Liu¹; Xiaofeng Wu¹; Yury O. Nunez Lopez²; Richard E. Pratley²; Anton B. Iluk^{1,3}; W. Andy Tao^{1,3}; ¹Purdue University, WEST LAFAYETTE, IN; ²AdventHealth, Orlando, FL; ³Tymora Analytical Operations, West Lafayette, IN
- MP 572 **A guide to high-throughput dose-resolved phosphoproteomics to understand drug mechanism(s) of action**; Florian P Bayer¹; Jana Zecha¹; Matthew The¹; Bernhard Kuster¹; ¹Technical University of Munich, Freising, Germany
- MP 573 **Three-dimensional construction of mouse brain protein atlas based on spatial multi-omics data**; Shuang Yang¹; Jing Yuan²; Huali Shen¹; Xiaohui Liu¹; ¹Fudan University, Shanghai, China; ²HuaZhong University of Science and Technology, Wuhan, China
- MP 574 **Streamlined protein extraction and cleanup for unbiasedly exploring pan-bacterial phosphoproteomics**; Pei-Shan Wu¹; Ting-An Chen¹; I-Ying Lin¹; Miao-Hsia Lin¹; ¹Department of Microbiology, College of Medicine, National Taiwan University, Taipei City, Taiwan
- MP 575 **A Bio-Zr based enrichment for the phosphopeptides from human and animal tissues**; Qidan Li¹; Xiaolian Ning¹; Zhoumei Zheng¹; Siqi Li¹; Ziyin Han¹; Jie Liu¹; Dongjie Wu¹; Zhanlong Mei¹; Jin Zi¹; Siqi Liu¹; ¹BGI-Shenzhen, Shenzhen, China
- MP 576 **High-throughput phosphoproteomics of formalin-fixed, paraffin-embedded rat tissues using microflow Zeno SWATH**; Erin M Humphries^{1,2}; Dylan Xavier¹; Keith Ashman³; Peter G Hains¹; Phillip J Robinson^{1,2}; ¹Children's Medical Research Institute, Westmead, Australia; ²University of Sydney, Sydney, Australia; ³SCIEX, Sydney, Australia
- MP 577 **Phospho-site identification of multiply phosphorylated tau peptides in human brain**; Gunnar Brinkmalm¹; Juan Lantero Rodriguez¹; Elena Camporesi¹; Laia Montoliu-Gaya¹; Johan Gobom¹; Ann Brinkmalm¹; Tammaryn Lashley²; Henrik Zetterberg¹; Kaj Blennow¹; ¹University of Gothenburg, Molndal, Sweden; ²University College London, London, United Kingdom
- MP 578 **Improving tryptic digestion efficiency for proteomic samples by metal ion additives**; Kosuke Ogata¹; Shunsuke Tanaka²; Ayana Tomioka¹; Eisuke Kanao^{1,3}; Yasushi Ishihama^{1,3}; ¹Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; ²Kyoto University, Kyoto, Japan; ³National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan
- MP 579 **Identifying MAPK signaling thresholds in melanoma using phosphoproteomics**; Kristyn R Hayashi^{1,2}; Natalie G Ahn^{1,2}; ¹Department of Biochemistry, University of

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- Colorado, Boulder, CO; ²BioFrontiers Institute, University of Colorado, Boulder, CO
- MP 580 **Phosphomatics V3: Expanding a web-based resource for online analysis of phosphoproteomics data;** Michael G Leeming¹; Ching-Seng Ang¹; Shuai Nie¹; Swati Varshney¹; Nicholas Williamson¹; ¹Melbourne Mass Spectrometry and Proteomics Facility, Bio21 Institute of Molecular Science and Biotechnology, The University of Melbourne, Parkville, Melbourne, Australia
- MP 581 **Digging deeper into phosphoproteomes through AI-driven deconvolution of chimeric spectra;** Florian Seefried¹; Daniel P. Zolg¹; Tobias Schmidt¹; Siegfried Gessulat¹; Michael Graber¹; Samia Ben Fredj¹; Patroklos Samaras¹; Markus Schneider¹; Layla Eljaghi¹; Vishal Sukumar¹; Pedro Navarro²; Kai Fritzscheier²; Yovany Cordero Hernandez²; Frank Berg²; Carmen Paschke²; David Horn²; Bernard Delanghe²; Christoph Henrich²; Martin Heinrich Frejno¹; ¹MSAID GmbH, Garching b.München, Germany; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- MP 582 **Quantitative phosphoproteomics to identify candidate target engagement biomarkers related to efferocytosis and TAM RTK pathways;** Manuel Tzouros¹; Emmanuelle Lezan¹; David Avila¹; Balazs Banfai¹; Florian Wanke²; Nicolas Mercado²; Barbara Geering²; ¹Roche Innovation Center Basel, Pharmaceutical Sciences, F. Hoffmann-La Roche, Ltd., Basel, Switzerland; ²Roche Innovation Center Basel, Immunology, Infectious Diseases and Ophthalmology (I2O) Discovery and Translational Area, F. Hoffmann-La Roche Ltd., Basel, Switzerland
- MP 583 **Phosphoproteomic analysis of the cellular response to lysosomal impairment;** Pathma Muthukottiappan¹; Alireza Dehghani¹; Asisa Muchamedin¹; Fatema Akter¹; Mariana Eca Guimaraes De Araujo²; Cristina Coman³; Robert Ahrends³; Lukas Huber²; Volkmar Gieselmann¹; Dominic Winter¹; ¹Institute for Biochemistry and Molecular Biology, Medical Faculty, Rheinische Friedrich-Wilhelms-University of Bonn, Bonn, Germany; ²Medical University of Innsbruck, Innsbruck, Austria; ³University of Vienna, Vienna, Austria
- MP 584 **Using large-scale phosphoproteomics to elucidate the regulation of Protein Kinase CK2 activity by peptidyl-prolyl cis/trans isomerase Pin1;** Scott E Roffey¹; David W Litchfield¹; ¹Western University, London, ON
- MP 585 **Quantitative analysis of phosphorylated proteins from multiple signaling pathways using the TMTpro and SureQuant targeted mass spectrometry assay panel reagents;** Ana Marcu¹; Bhavin Patel²; Jae Choi²; Dustin Frost²; Penny Jensen²; Airmansoor Hakimi³; Kay Opperman²; Ryan Bomgarden²; Christopher M Rose¹; ¹Genentech Inc., South San Francisco, CA; ²Thermo Fisher Scientific, Rockford, IL; ³Thermo Fisher Scientific, San Jose, CA
- MP 586 **Characterizing the effects of kinase inhibitors on the phosphorylation of transcription factors using subcellular fractionation;** Andrea I Gutierrez¹; Isabella T Whitworth²; Carolyn Allen¹; William E Fondrie¹; Daniele Canzani¹; Lindsay K Pino¹; Alexander J Federation¹; ¹Talus Bioscience, Seattle, WA; ²University of Wisconsin-Madison, Madison, WI
- MP 587 **Multi-species Benchmarking Phospho-DIA Comparison of Commercial Sample Prep Kits;** Billy W Newton¹; Audrick Yang¹; Ying Zhu¹; Guanghui Han¹; ¹BGI Americas, San Jose, CA
- MP 588 **Advancements in phosphopeptide elucidation is possible: permethylation via TrEnDi improves LCMS detection of phosphopeptides;** Samiksha Vij¹; Karl Wasslen¹; Jeffrey M Manthorpe¹; Jeffrey C Smith¹; ¹Carleton University, Department of Chemistry, Ottawa, ON
- MP 589 **Characterizing Root Exudate Composition Across 19 Cover Crop Species;** Valerie Seitz¹; Colorado State University, Fort Collins, CO
- MP 590 **GC-MS Profiling of Compounds Present in the Endangered Plant *Ziziphus celata*;** Emily Boyette¹; Luc Alfred¹; Sarah Arnan¹; Toby Ellison¹; Jenna Gutierrez¹; Stephanie Hicks¹; Nylla Wilder¹; Kate Calvin¹; ¹South Florida State College, Avon Park, FL
- MP 591 **A Suspension Trapping-based Sample Preparation Workflow for Sensitive Plant Phosphoproteomics;** Chin-Wen Chen¹; Chia-Feng Tsai²; Shu-Yu Lin³; Chuan-Chih Hsu¹; ¹Institute of Plant and Microbial Biology, Academia Sinica, Taipei city, Taiwan; ²Pacific Northwest National Laboratory, Richland, WA; ³Academia Sinica Common Mass Spectrometry Facilities for Proteomics and Protein Modification Analysis, Academia Sinica, Taipei, Taiwan
- MP 592 **Quantitative proteomic analysis of rice plants with different phosphorus use efficiency phenotypes when grown in low and high phosphorus conditions;** Yoshiaki Ueda¹; Farhad Massomi-Aladizgeh²; M. Asaduzzaman Proadhan³; Mehdi Mirzaei²; Ghasem Hosseini Salekdeh²; Matthias Wissuwa¹; Paul A. Haynes²; ¹Japan International Research Center for Agricultural Sciences (JIRCAS), Tsukuba, Japan; ²Macquarie University, North Ryde, Sydney, Australia; ³University of Western Australia, Perth, Australia
- MP 593 **The Detection by High Resolution Mass Spectrometry of Mogrosides Produced Through Metabolic Engineering of Diverse Plant Species;** Matthew B. Kilgore¹; Anna Matthiadis¹; Devarshi Selote¹; Jack Wilkinson¹; ¹Elo Life Systems, Durham, NC
- MP 594 **Extending a Tandem Mass Spectral Library with High-Quality Reference Spectra of 11,000 Plant Metabolites;** Xiaoyu Yang¹; Pedatsur Neta¹; H. Martin Garraffo¹; Yuxue Liang¹; Yamil Simón-Manso¹; Yi Liu¹; Dmitrii V. Tchekhovskoi¹; Yuri A. Mirokhin¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD
- MP 595 **Metabolomics Revealed the Roles of Oxylipins and Melatonin in Stomatal Immunity;** Qingyuan Xiang¹; Craig Dufresne²; Sixue Chen^{1,3}; ¹Department of Biology, Genetics Institute, University of Florida, Gainesville, FL; ²Thermo Scientific Training Institute, West Palm Beach, Florida; ³Department of Biology, University of Mississippi, Oxford, MS
- MP 596 **Comprehensive Lipidome Survey of the Tomato Suffered from Distinct Infection Phases of Late Blight Disease;** Chia-Wei Hsu^{1,2}; Yet-Ran Chen^{1,2}; ¹Academia Sinica, Taipei, Taiwan; ²Academia Sinica Metabolomics Core Facility, Taipei, Taiwan
- MP 597 **Dimensionality reduction methods and GNPS for plant metabolomics of *Centella asiatica* cultivars;** Luke C Marney^{1,2}; Md Alam Nure^{1,2}; Liping Yang^{1,2}; Jaewoo Choi^{2,3}; Natasha Cerruti^{2,4}; Armando Magana^{1,2,3}; Corey De la Cruz⁵; Gerrad Jones⁵; Kadine Cabey^{2,6}; Ramya Viswanathan^{2,6}; Sumanaa Rajagopal^{2,6}; James Smith⁷; Amala Soumyanath^{2,6}; Jan F. Stevens^{2,3,8}; Claudia Maier^{1,2,3}; ¹Department of Chemistry, Oregon State University, Corvallis, OR; ²BENFRA Botanical Dietary Supplements Research Center, Oregon Health and Science University, Portland, OR; ³Linus Pauling Institute, Oregon State University, Corvallis, OR; ⁴Oregon Wild Harvest, Redmond, OR; ⁵Biological & Ecological Engineering, Oregon State University, Corvallis, OR; ⁶Department of Neurology, Oregon Health & Science University, Portland, Oregon; ⁷School of Food Science & Nutrition, University of Leeds, Leeds, United Kingdom; ⁸Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR
- MP 598 **From exploratory analysis to high-throughput quantitative analysis of *Withania somifera* extract using LC-HRMS/MS and LC-MRM-MS;** Luke Marney^{1,2}; Jaewoo Choi^{2,3}; Armando Alcazar Magana^{1,2,3}; Liping Yang^{1,2}; Md Alam Nure^{1,2}; Mikah Brandes^{2,4}; Cody Neff^{2,4}; Amala Soumyanath^{2,5}; Jan Frederik Stevens^{2,3,6}; Claudia Maier^{1,2,3}; ¹Department of Chemistry, Oregon State University, Corvallis, OR; ²BENFRA Botanical Dietary Supplements Research Center, Oregon Health and Science University, Portland, OR; ³Linus Pauling Institute, Oregon State University, Corvallis, OR; ⁴Department of Neurology,

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- MP 599 **Plant Proteomic Response to Complex Microbial Community Topsoil Inoculation**; Brandon A Saiz¹; Linda Van Diepen¹; Franco Basile¹; Rachel Standish²; ¹University of Wyoming, Laramie, WY; ²Murdoch University, Perth, Australia
- MP 600 **Inside into the proteome of *Chelidonium majus* latex**; Joanna Gracz-Bernaciak¹; Oliwia Mazur¹; Natalia Kielich¹; Michalina Krakowiak¹; Sophia Baldysz¹; Martyna Węglewska¹; Oskar Musidlak¹; Agata Malinowska²; Robert Nawrot¹; ¹Adam Mickiewicz University in Poznan, Faculty of Biology, Department of Molecular Virology, Poznan, Poland; ²Polish Academy of Sciences, Institute of Biochemistry and Biophysics, Mass Spectrometry Laboratory, Warsaw, Poland
- MP 601 **Protein network analysis and metabolite correlation reveals primary metabolism contribution to susceptibility or resistance of *Eucalyptus grandis* to rust**; Thais Regiani Cataldi¹; Ana Lúcia Mendes Pinheiro¹; Felipe Garbelini Marques¹; Alline Sekiya¹; Fabrício Edgar De Moraes¹; Carlos Alberto Labate¹; ¹ESALQ, Piracicaba, Brazil
- MP 602 **Diversity and Antifungal Activity of Specialized Metabolites in Ecotypes of the Bioenergy Crop Switchgrass (*Panicum virgatum* L.)**; Xingxing Li^{1,2}; Ming-Yi Chou^{1,3}; Gregory Bonito^{1,3}; Arthur Daniel Jones^{1,2}; Robert L. Last^{1,2,4}; ¹DOE Great Lakes Bioenergy Research Center, Michigan State University, East Lansing, MI; ²Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI; ³Department of Plant, Soil and Microbial Sciences, Michigan State University, East Lansing, MI; ⁴Department of Plant Biology, Michigan State University, East Lansing, MI
- MP 603 **Achieving higher productivity in cell line optimization by a streamlined middle-down workflow**; Hirsh Nanda¹; Andrew Mahan¹; Zoe Zhang²; Partha Chowdhury¹; ¹Janssen Research & Development, Spring House, PA; ²SCIEX, Redwood city, CA
- MP 604 **Standard-Free Absolute Quantitation of Antibody Deamidation Degradation and Host Cell Proteins by Coulometric Mass Spectrometry**; Yongling Ai¹; Harsha P. Gunawardena²; Xuanwen Li³; Yong-Ick Kim¹; Howard D. Dewald⁴; Hao Chen¹; ¹New Jersey Institute of Technology, Newark, NJ; ²Janssen Research & Development, Spring House, PA; ³Analytical Research & Development, Merck & Co., Inc., Kenilworth, NJ; ⁴Ohio University, Athens, OH
- MP 605 **Top Down Analysis of a Multivalent PEGylated Fab-based Biotherapeutic in Cynomolgus Plasma to Assess in vivo Biotransformation using IA-LC-TOF-MS**; Sylvia C Wong¹; M. Violet Lee¹; Ola Saad¹; ¹Genentech Inc., South San Francisco, CA
- MP 606 **Newomics® Microflow- Nanospray ESI-MS (Mn3ESI-MS) Platform for Sensitive and Robust Analysis of Monoclonal Antibody Glycoforms**; Nancy Fernandes; Lonza, Portsmouth, NH
- MP 607 **Recombinant chymotrypsin for improved peptide mapping of biotherapeutic proteins**; Alba Katiria González Rivera¹; Sergei Saveliev¹; Michael M. Rosenblatt¹; Ethan Strauss¹; Matt Larsen¹; Evan Hsu¹; John Van Herwynen¹; Marjeta Urh¹; ¹Promega Corporation, Madison, WI
- MP 608 **Peptide Mapping of a Monoclonal Antibody Using an Integrated Protein Digestion LCMS Platform (Perfinity-QTOF LCMS-9030)**; Kate (xiaomeng) Xia¹; Evelyn H. Wang¹; Stephen Kurzyniec¹; Tairo Ogura¹; Yoshiyuki Okamura¹; Mohamed Boutaghou¹; ¹Shimadzu Scientific Instruments, Columbia, MD
- MP 609 **A Novel Approach to Mass Spec Sample Preparation of AAV Capsid Protein for Peptide Mapping and Host Cell Impurity analysis**; Sergei Saveliev¹; Chris Hosfield¹; Alba Katiria González Rivera¹; Marjeta Urh¹; Michael M. Rosenblatt¹; ¹Promega Corporation, Madison, WI
- MP 610 **Effect of in-Source CID on non-Specific truncation in Characterization of Antibody-based Therapeutics using Reduced LC-MS Analysis**; Roshanak Aslebagh¹; Kai Zheng¹; ¹CytomX Therapeutics, South San Francisco, CA
- MP 611 **Intact Mass Analysis of Biotherapeutic Stability in Tissues**; Yunan Wang¹; Mei Han¹; Justin Iwuagwu¹; Fang Xie¹; Lin Zeng¹; Kip Conner¹; ¹Amgen, Inc., South San Francisco, CA
- MP 612 **Enhanced biopharmaceutical characterization using next generation multireflecting time-of-flight technology**; Guillaume Bechade¹; Dale A Cooper-Shepherd²; Emma Marsden-Edwards²; Martin E. Palmer²; ¹Waters S.A.S, Saint-Quentin, France; ²Waters Corporation, Wilmslow, United Kingdom
- MP 613 **Characterization of carbamoylated lysine in a therapeutic recombinant protein top-down electron fragmentation**; Joaquín Barbeito¹; Rachel Franklin²; Joseph Meeuwssen²; Mike Hare²; Yury Vasil'ev²; Joseph Beckman²; ¹Xeptiva, Montevideo, Uruguay; ²e-MSon, Corvallis, OR
- MP 614 **Monitoring mAb proteoforms in mouse plasma using an automated immunocapture combined with top-down and middle-down mass spectrometry**; Jonathan Dhenin^{1,2,3}; Valérie Lafont²; Mathieu Dupré²; Norbert Zombori²; Alain Krick²; Christine Mauriac²; Julia Chamot-Rooke^{1,3,4}; ¹Institut Pasteur, Paris, France; ²Sanofi, Chilly-Mazarin, France; ³Université Paris Cité, Paris, France; ⁴CNRS, Paris, France
- MP 615 **Characterization of Charge Variants by Ion Exchange Chromatography and Mass Spectrometry**; Yun Zhang¹; Li-I Tsao¹; Tiffany Hawkins¹; Brian Woodrow¹; ¹MilliporeSigma, Rockville, MD
- MP 616 **"Flash Characterization" of Antibodies via Microdroplet Reactions in an Unmodified Jet Stream Source**; Michael D Knierman¹; Jim Lau²; Hui Zhao²; Harsha P. Gunawardena³; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, Wilmington, DE; ³Janssen Research & Development, Spring House, PA
- MP 617 **Chemical labeling and mass spectrometry for characterization of the higher-order structure of a bispecific antigen-binding biotherapeutic (BABB) and its complexes**; Arnik Shah^{1,2}; Dipa Batabyal³; Dayong Qiu¹; Weidong Cui¹; John Harrahy^{1,4}; Alexander R. Ivanov²; ¹Amgen Inc., Cambridge, MA; ²Northeastern University, Boston, MA; ³Amgen, Thousand Oaks, CA; ⁴Sanofi, Cambridge, MA
- MP 618 **Multi-attribute method (MAM) for biotherapeutics characterization: biosimilarity assessment, high-throughput and low-flow analytical methods applications**; Silvia Millan Martin¹; Craig Jakes¹; Lisa Strasser¹; Sara Carillo¹; Jonathan Bones^{1,2}; ¹NIBRT, Dublin, Ireland; ²University College Dublin, Belfield, Ireland
- MP 619 **Peptide mapping workflow for direct microchip CE-MS analysis of biopharmaceuticals**; Sara Carillo¹; Rachel Ronan¹; Adi M Kulkarni²; Erin Redman³; Kate Yu²; Jonathan Bones¹; ¹Characterization and Comparability Laboratory, NIBRT, Dublin, Ireland; ²908 Devices, Inc., Boston, MA; ³908 Devices, Inc., Carboro, NC
- MP 620 **Mass spectrometry-based approaches to investigate allosteric modulation and biased signaling of GPCR's**; Parth Kapoor¹; Ildir Liko¹; Fernando Almeida¹; Jonathan Hopper¹; Joanna Toporowska²; Argyris Politis³; Hsin-yung Yen⁴; ¹OMass Therapeutics, Oxford, United Kingdom; ²King's College London, London, United Kingdom; ³University of Manchester, Manchester, United Kingdom; ⁴Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan
- MP 621 **Development of Multi-Attribute method (MAM) for heavily glycosylated protein vaccines**; Asif Shaijahan¹; Vera B. Ivleva¹; Jason G. Gall¹; Q. Paula Lei¹; ¹Vaccine

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- MP 622 **Novel approach to achieve high spectral quality without compromising identification for biopharma applications;** Stephane Houel¹; Sara Carillo²; Craig Jakes²; Silvia Millán-Martín²; Segá Ndiaye³; Kevin L Schauer¹; Jonathan Bones²; Shannon Eliuk¹; ¹ThermoFisher Scientific, San Jose, CA; ²NIBRT, Dublin, Ireland; ³Thermo Fisher Scientific, Courtaboeuf, France
- MP 623 **In Vivo Structural Analysis of Membrane Proteins via Hydroxyl Radical Footprinting;** James Dowell¹; Daniel Benjamin¹; Faraz Choudhury¹; ¹Immuto Scientific, Madison, WI
- MP 624 **Investigations of a Bispecific Antibody Dimerization via Hydroxyl Radical Footprinting;** Harsha Gunawardena¹; Andrew Mahan¹; Hirsh Nanda¹; Daniel Benjamin²; ¹JOHNSON AND JOHNSON, Spring House, PA; ²Immuto Scientific Inc., Madison, WI
- MP 625 **A native multi-dimensional MAM workflow for at-line characterization of mAb titer, size, charge, and glycoform heterogeneities in cell culture supernatant;** Sanghati Bhattacharya¹; Srishiti Joshi¹; Anurag Singh Rathore¹; ¹Indian Institute of Technology, Delhi, Delhi, India
- MP 626 **Multi-attribute monitoring of aggregates and charge variants of monoclonal antibody through native 2D-SEC-MS-WCX-MS;** Sunil Kumar¹; Tushar Sharad Savane²; Vadiraja Bhat³; Anurag Singh Rathore²; ¹Indian Institute of Technology Delhi, New Delhi, India; ²Indian Institute of Technology, Delhi, New Delhi, India; ³Agilent Technologies, Bangalore, India
- MP 627 **A Disruptive Approach for Characterization of mAb Charge Variants by Imaged Capillary Isoelectric Focusing (icIEF)-UV/MS;** Greg Adams¹; Hunter Walker¹; Margo Wilson¹; Scott Mack²; Maggie Ostrowski²; ¹FUJIFILM Diosynth Biotechnologies USA, Morrisville, NC; ²SCIEX, Fremont, CA
- MP 628 **Top/Middle-Down Protein Sequencing: a novel automated data processing tool for the Top-Down/Middle-Down analysis of biological therapeutics;** Mona Hamada¹; Stefano Gotta²; Wen Jin¹; Amy Claydon³; Amandine Boudreau¹; ¹SCIEX, Concord; ²Genedata, Basel, Switzerland; ³Genedata, Cambridge, United Kingdom
- MP 629 **A Single Data Workflow Leveraging Middle-Down Sequencing to Validate Intact Mass Analysis Characterization of Therapeutic Antibodies;** Stephen Kok¹; Maurizio Bronzetti¹; Aude Tartiere¹; Amy Claydon²; Arnd Brandenburg³; ¹Genedata, San Francisco, CA; ²Genedata, Cambridge, United Kingdom; ³Genedata, Basel, Switzerland
- MP 630 **Rapid analysis of titre, aggregate and intact mass of antibody therapeutics using multi-dimensional liquid chromatography coupled with native mass spectroscopy;** Tushar Sharad Savane¹; Sunil Kumar²; Vadiraja Bhat³; Anurag Singh Rathore¹; ¹Indian Institute of Technology Delhi, New Delhi, India; ²Indian Institute of Technology Delhi, New Delhi, India; ³Agilent technologies, Bangalore, India
- MP 631 **Investigating the conformational dynamics of the interprotein calmodulin-nitric oxide synthase complex by cross-linking mass spectrometry;** Ting Jiang¹; Guanghua Wan¹; Haikun Zhang¹; Eric Underbakke²; Changjian Feng¹; ¹UNM College of Pharmacy, Albuquerque, NM; ²Roy J. Carver Department of Biochemistry, Biophysics and Molecular Biology, Ames, Iowa
- MP 632 **Mass Spectrometric Recognition Motif Discovery by Intact Transition Epitope Mapping – Force differences between Original and Unusual Residues (ITEM-FOUR) Analysis;** Claudia Röwer¹; Christian Ortmann²; Andrei Neamtu³; Reham F. El-Kased⁴; Michael O. Glocker¹; ¹Proteome Center Rostock, Rostock, Germany; ²Waters Corporation - TA Instruments, Eschborn, Germany; ³TRANSCEND Centre, Regional Institute of Oncology (IRO) Iasi, Iasi, Romania; ⁴The British University in Egypt, El Sherouk City, Egypt
- MP 633 **Identification and structural modeling of the nuclear receptor liver receptor homolog-1 with a novel corepressor peptidylprolyl cis/trans isomerase B;** Valentine V Courouble^{1,2}; Bilel Bdiri¹; Roberto Vera Alvarez³; Bruce D Pascal³; Theodore Kamenecka¹; Patrick R. Griffin^{1,2}; ¹The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL; ²Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; ³Omics Informatics, Honolulu, HI
- MP 634 **Examining the Structure-Function Relationship of Enzymes using Temperature-Controlled Nanoelectrospray Mass Spectrometry;** Julian Alexander Harrison¹; Adam Pruška¹; Renato Zenobi¹; ¹ETH Zurich, Zurich, Switzerland
- MP 635 **Limited proteolysis-mass spectrometry (LiP-MS) enables global profiling of the effects of glycosylation on protein conformational changes;** Haiyan Lu¹; Xudong Shi²; Lauren Fields³; Hua Zhang¹; Danqing Wang³; Nathan V. Welham²; Lingjun Li¹; ¹School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ²School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; ³Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- MP 636 **Understanding the role of conformational dynamics in the substrate promiscuity of the Pup-proteasome system in mycobacteria;** Alicia Plourde¹; Siavash Vahidi¹; ¹University of Guelph, Guelph, ON
- MP 637 **Tracking the Mechanistic Origins of Irreversible Protein Unfolding;** Evelyn H MacKay-Barr¹; Lars Konermann¹; ¹University of Western Ontario, London, ON
- MP 638 **Determining Collision Cross Sections Using Orbitrap Charge Detection Mass Spectrometry;** Kyle Patrick Bowen¹; Michael Senko¹; ¹Thermo Fisher Scientific, San Jose, CA
- MP 639 **Establishing a decision tree for native mass spectrometry analysis of membrane proteins in complex membrane mimetics;** Weijing Liu¹; Christopher Mullen¹; Donggyun Kim²; Vadim Cherezov²; Gregory J Dodge³; Barbara Imperiali³; Hiruni S. Jayasekera⁴; Michael T Marty⁴; Rosa Viner¹; ¹Thermo Fisher Scientific, San Jose, CA; ²University of Southern California, Los Angeles, CA; ³Massachusetts Institute of Technology, Cambridge, MA; ⁴University of Arizona, Tucson, AZ
- MP 640 **Monitoring of conformational changes in transmembrane proteins using HDX and FFAP radical labeling;** Lukáš Fojtík^{1,2}; Jasmína Portašiková^{1,2}; Petr Pompach^{2,3}; Zdeněk Kukačka¹; Petr Novák^{1,2}; Petr Man^{1,2}; ¹Institute of Microbiology of the CAS, v. v. i., Prague, Czech Republic; ²Charles University, Faculty of science, Prague, Czech Republic; ³Institute of Biotechnology of the CAS, v. v. i., Prague, Czech Republic
- MP 641 **Characterizing Macromolecular Dipole Moments via Differential Ion Mobility Spectrometry with Linked Field/Pressure Scans;** Alexandre A Shvartsburg¹; Roch Andrzejewski²; Andrew Entwistle²; Monika Gomola²; Patrick Knight²; ¹Wichita State University, Wichita, KS; ²Shimadzu Research Laboratory (Europe), Manchester, United Kingdom
- MP 642 **Altered dimerization kinetics and dynamics of SARS-CoV-2 main protease determined by native and hydrogen-deuterium exchange mass spectrometry;** Syuan-Ting Kuo¹; Yan Xin¹; David Russell¹; ¹Texas A&M, College Station, TX
- MP 643 **Dysregulation of mitochondrial ClpP protease using orthosteric and allosteric inhibitors;** Monica M Goncalves¹; Angelina S Kim¹; Algirdas Velyvis¹; Taylor Forrester¹; Vincent Trudel²; Matthew Kimber¹; Aaron Schimmer³; Andrei Yudin²; Siavash Vahidi¹; ¹University of Guelph, Guelph, ON; ²University of Toronto, Toronto, ON;

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- MP 644 **Cryo-EM atomic structure determination from macromolecular samples produced by native electrospray ion beam deposition (ESIBD);** Tim K Esser¹; Jan Bohning²; Paul Fremdling³; Carol V Robinson³; Justin L. P. Benesch³; Lindsay Baker³; Tanmay A.M. Bharat²; Stephan Rauschenbach⁴; ¹University of Oxford, Oxford, United Kingdom; ²Structural Studies Division, MRC Laboratory of Molecular Biology, Cambridge, United Kingdom; ³Oxford University, Oxford, United Kingdom; ⁴University of Oxford, Dept. of Chemistry, Oxford, United Kingdom
- MP 645 **Structural interactomics and structure predictions reveal protein binding sites within disordered regions;** Julia Ruta¹; Cong Wang¹; Ying Zhu¹; Pin-Lian Jiang¹; Arne Elofsson^{2,3}; Boris Bogdanow¹; Fan Liu^{1,4}; ¹Department of Structural Biology, Leibniz Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; ²Department of Biochemistry and Biophysics, Stockholm University, Stockholm, Sweden; ³Science for Life Laboratory, Stockholm University, Solna, Sweden; ⁴Charité – Universitätsmedizin Berlin, Berlin, Germany
- MP 646 **Structural investigation of large eye lens β -crystallin heterooligomers using native ion mobility-mass spectrometry and computations;** Micah T Donor¹; Amber Rolland^{2,3}; Takumi Takata⁴; Kirsten J Lampi⁵; James S. Prell³; ¹George Fox University, Newberg, OR; ²Utrecht University, Utrecht, Netherlands; ³University of Oregon, Department of Chemistry and Biochemistry, Eugene, OR; ⁴Kyoto University, Kyoto, Japan; ⁵Oregon Health & Science University, Portland, Oregon
- MP 647 **Reactivity of proteins with singlet molecular oxygen as a probe for structural mass spectrometry;** Michael Volny^{1,2}; Giovanni Tonnizzo^{1,3}; Marek Polák^{1,2}; Lukáš Fojtík^{1,2}; Daniel Kavan^{1,2}; Petr Man^{1,2}; Petr Novák^{1,2}; ¹Charles University, Faculty of Science, Prague, Czech Republic; ²BioCeV - Institute of Microbiology, Prague, Czech Republic; ³University of Padua, Department of Pharmacy, Padua, Italy
- MP 648 **Supercharging reagent improves nanoHPLC-ESI-MS/MS analysis of disulfide bonds and His-tagged peptides;** Chia-Wei Lin¹; Fabia Canonica²; Simone Wüthrich¹; Paolo Nanni¹; Ralph Schlapbach¹; ¹Functional Genomics Center Zurich, University of Zurich & ETH Zurich, Zurich, Switzerland; ²Department of Dermatology, University of Zurich, Zurich, Switzerland
- MP 649 **Millisecond time-resolved hydrogen/deuterium-exchange mass spectrometry at single amino acid resolution resolves conformers of α -synuclein familial mutants;** Lindsay Cole¹; Ulrik H Mistrar²; Andrew J K Williamson³; Ken Cook³; Jenny Ho³; Yuqi Shi⁴; Rosa Viner⁴; Jonathan J Phillips⁵; ¹Applied Photophysics Ltd, Leatherhead, United Kingdom; ²Thermo Fisher Scientific, Copenhagen, Denmark; ³Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; ⁴ThermoFisher Scientific, San Jose, CA; ⁵Living Systems Institute, University of Exeter, Exeter, United Kingdom
- MP 650 **Application of a Benchtop Method for Oxidative Footprinting to Detect Structural Changes in a Protein Complex from *Staphylococcus Aureus*;** Maria C Panepinto¹; Juliana Ilmain¹; Victor Torres¹; Beatrix Ueberheide¹; ¹NYU Grossman School of Medicine, New York, NY
- MP 651 **Investigating binding interactions between SARS-CoV-2 PLpro and inhibitors, interferons and viral targets using ultraviolet photodissociation and collision cross section analysis;** Virginia K. James¹; Katelynn S. Zuercher¹; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- MP 652 **Characterization of loading efficiency of protein nanocages with native MS and limited charge reduction;** Kevin Cheung¹; Daniil G Ivanov¹; Igor A Kaltashov¹; ¹University of Massachusetts at Amherst, Amherst, MA
- MP 653 **Mapping the C-terminus of α -Synuclein conformers by native crosslinking and ion mobility mass spectrometry;** Melanie Cheung See Kit¹; Ian K. Webb¹; ¹Indiana University Purdue University Indianapolis, Indianapolis, IN
- MP 654 **Insights into the Fission Yeast Rhp6, Brl1 and Brl2 Complex using Crosslinking-MS;** Enrique Arevalo¹; Chu Thet Ywe¹; Sara Magoun¹; Jonathan Garcia¹; Prakash K. Shukla²; Mahesh B. Chandrasekharan²; ¹Spectrus, Beverly, MA; ²Department of Radiation Oncology and Huntsman Cancer Institute, University of Utah School of Medicine, Salt Lake City, Utah
- MP 655 **Variable-Temperature Electrospray Ionization Coupled with Electron Capture Dissociation to Study Temperature Induced Solution Phase Structural Changes;** Kristie L Baker¹; Philip C Lacey¹; Yuan Gao¹; Benjamin J. Jones¹; Vicki H Wysocki¹; ¹The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH
- MP 656 **Assay for solvent accessibility of methionine residues in complex sample using methionine oxidation footprinting and top-down proteomics;** Anju Teresa Sunny¹; Yanting Guo¹; Kellye A Cupp-Sutton¹; Si Wu¹; ¹University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK
- MP 657 **Mass spectrometry-based structural investigations of S100b;** Nolan K McLaughlin¹; Nicole D. Wagner¹; Michael L. Gross^{1,2}; ¹Washington University in Saint Louis, Saint Louis, MO; ²Washington University School of Medicine, St. Louis, MO
- MP 658 **Aggregation pathways of Transthyretins: a mass spectrometry study on health-related mutants;** Liqi Fan¹; David H. Russell¹; ¹Texas A&M University, College Station, TX
- MP 659 **Monitoring MsbA Activity under Turnover Conditions;** Tianqi Zhang¹; Jixing Lyu¹; Arthur Laganowsky¹; ¹Texas A&M University, College Station, TX
- MP 660 **Enabling simultaneous photoluminescence spectroscopy and X-ray Footprinting to study protein conformation and interactions;** Sayan Gupta¹; Line G Kristensen¹; Brandon Russell¹; Shawn M Costello²; Susan Marqusee²; Corie Y Ralston¹; ¹Lawrence Berkeley National Laboratory, Berkeley, CA; ²University of California, Berkeley, CA
- MP 661 **AlphaCross-XL: A rapid and robust tool for the identification of cross-linking of proteins using XL-MS;** Deeptarup Biswas¹; Sanjyot Vinayak Shenoy¹; Kamal Mandal²; Arthur Zalevsky²; Ayushi Verma¹; Audrey Kishishita²; Andrej Sali²; Sanjeeva Srivastava^{1,2}; Arun P. Wiita²; ¹IIT Bombay, Mumbai, India; ²UCSF, San Francisco, CA
- MP 662 **Electrochemical Oxidation-State Switching of Heme in Cytochrome c Reveals Associated Covalent Modifications.;** Pablo Scrosati¹; Lars Konermann¹; ¹Western University, London, ON
- MP 663 **Enzyme-based arginylome discovery in whole proteomes using isotopic labeling;** Zongtao Lin¹; Joanna M Gongora¹; Yixuan (axe) Xie¹; Samaneh G. Kondalaji¹; Xingyu Liu¹; Mingzhou Zhou¹; Faith M Robison¹; Dongwen Lv²; Anna S. Kashina³; Michael J. Greenberg¹; Benjamin A Garcia¹; ¹Washington University in St. Louis, St. Louis, MO; ²University of Texas Health Science Center at San Antonio, San Antonio, Texas; ³University of Pennsylvania, Philadelphia, PA
- MP 664 **Identification of 113 new histone marks by CHiMA, a tailored database search strategy;** Jinjun Gao¹; Xinlei Sheng¹; Jianfeng Du¹; Di Zhang²; Chang Han¹; Yue Chen³; Chu Wang²; Yingming Zhao¹; ¹The University of Chicago, Chicago, IL; ²Peking University, Beijing, China; ³University of Minnesota, Minneapolis, MN

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- MP 665 **Integrating mass spectrometry and icIEF: a state of the art technology for high-resolution characterization of protein charge heterogeneity**; Teresa Kwok¹; Mike Zhou¹; She Lin Chan¹; Anna Schaefer¹; Xiaoxi Zhang²; Min Du³; ¹Advanced Electrophoresis Solutions Ltd., Cambridge, ON; ²Thermo Fisher Scientific, Shanghai, China; ³Thermo Fisher Scientific, Boston, MA
- MP 666 **Engineering an enzymatic tool for chemoselective C-terminal modification**; Clara Frazier¹; Amy Weeks¹; ¹Biochemistry, University of Wisconsin Madison, Madison, WI
- MP 667 **An in situ chemically-induced modular strategy to profile E2-dependent ubiquitination events in living cells**; Suprama Datta¹; Caitlin J. Hill¹; Nicholas P. McCurtin¹; Rebecca A. Scheck¹; ¹Tufts University, Medford, MA
- MP 668 **The regulation and functions of lysine lactylome in Escherichia coli**; Hanyang Dong¹; Jianji Zhang¹; Kai Zhang¹; ¹Tianjin Medical University, Tianjin, China
- MP 669 **Utilizing SILAC Labeled Immunoglobulins for the Absolute and Relative Quantification of Glycation and Other PTMs**; Sonal Priya¹; Ron Orlando¹; Marla Popov²; ¹University of Georgia, Athens, GA; ²Glycoscientific, Athens, GA
- MP 670 **Identification and differentiation of positional isomers of O-linked glycopeptides of etanercept using an alternative electron-based MS/MS approach**; Zoe Zhang¹; Haichuan Liu²; Xuezhi Bi³; ¹Sciex, Redwood City, CA; ²SCIEX, Redwood city, CA; ³Bioprocessing Technology Institute (BTI), Singapore, Singapore
- MP 671 **A single-injection workflow for enhanced peptide mapping using collision-induced dissociation (CID) and electron activated dissociation (EAD)**; Elliott Jones; ¹Sciex, Redwood City, CA
- MP 672 **Ion Mobility Separations of Largest Peptide Epimers and Intact Isomeric Proteoforms with Variant PTM Localizations**; Gayani Wijegunawardena¹; Hayden A Thurman¹; Francis Berthias²; David Williamson³; Haifan Wu¹; Gabe Nagy³; Ole Jensen²; Alexandre A Shvartsburg¹; ¹Wichita State University, Wichita, KS; ²Southern Denmark University, Odense, Denmark; ³University of Utah, Salt Lake City, UT
- MP 673 **Redox proteomics of how Trx1 promotes autophagy through transnitrosylation of Atg7 during myocardial ischemia**; Narayani Nagarajan¹; Shinichi Oka¹; Tong Liu¹; Hong Li¹; Junichi Sadoshima¹; ¹Rutgers New Jersey Medical School, Newark, NJ
- MP 674 **Revealing non-canonical phosphorylation of the SARS-CoV-2 nucleocapsid serine/arginine-rich domain using top-down electron capture dissociation and sequence tag generation**; Rachel Franklin^{1,2}; Phillip Zhu¹; Adrian Guthals²; Joseph Meeuwssen²; Stephen Madden²; Michael C. Hare²; Richard Cooley³; Joseph Beckman²; ¹Oregon State University, Corvallis, OR; ²e-MSion, Corvallis, OR; ³Oregon State University, Corvallis
- MP 675 **Exploring multiplexing strategies for ADP-Ribosylation**; Martin Rykar¹; Holda Awah Anagho¹; Ivo A Hendriks¹; Michael L Nielsen¹; ¹University of Copenhagen, Copenhagen, Denmark
- MP 676 **A mass spectrometric based characterization of protein aggregates isolated from a cohort of Progressive Supranuclear Palsy patients**; Maaïke Beuvinck¹; Mukesh Kumar¹; Arthur Viode¹; Christoph N Schläffner¹; Kathrin Wenger¹; Timothy Chang²; Michael Deture³; Daniel Geschwind²; Dennis W Dickson³; Hanno Steen¹; Judith Steen¹; ¹Boston Childrens Hospital, Boston, MA; ²UCLA Mednet, Los Angeles, CA; ³Mayo Clinic, Rochester, MN
- MP 677 **Site-specific Detection of Protein S-acylation by IodoTMT Labeling and Immobilized anti-TMT Antibody Resin Enrichment**; Jian Cai¹; Ming Song²; Ming Li¹; Michael Merchant³; Frederick Benz⁴; Jon Klein^{1,5}; Craig McClain^{2,6,7,8}; ¹Division of Nephrology and Hypertension, Department of Medicine, University of Louisville School of Medicine, Louisville, Kentucky; ²Division of Gastroenterology, Hepatology and Nutrition, Department of Medicine, University of Louisville School of Medicine, Louisville, KY; ³Division of Nephrology and Hypertension, Department of Medicine, University of Louisville School of Medicine, Louisville, KY; ⁴Department of Pharmacology and Toxicology, University of Louisville School of Medicine, Louisville, KY; ⁵Robley Rex Veterans Affairs Medical Center, Louisville, Kentucky; ⁶Alcohol Research Center, University of Louisville, Louisville, KY; ⁷Hepatobiology and Toxicology Center, University of Louisville, Louisville, KY; ⁸Robley Rex Veterans Affairs Medical Center, Louisville, KY
- MP 678 **Global succinylome and proteome of human brain reveal succinylation of key lysine residues of hallmark proteins associated with Alzheimer's disease**; Elizabeth T Anderson¹; Yun Yang²; Victor Tapias²; Hui Xu²; Ruchika Bhawal¹; Qin Fu¹; Gary E. Gibson²; Sheng Zhang¹; ¹Proteomics and Metabolomics Facility, Cornell University, Ithaca, NY; ²Burke Neurological Institute, Weill Cornell Medicine, White Plains, NY
- MP 679 **BioPlexPTM: Linking Cell-Specific Interactions to Differential Protein Expression and Post-Translational Modifications**; David R Vanderwall¹; Brandon Gassaway¹; Laura Pontano Vaites¹; David P Nusinow²; Donald S Kirkpatrick²; J. Wade Harper¹; Steven P Gygi¹; Edward L Huttlin¹; ¹Harvard Medical School, Boston, MA; ²Interline Therapeutics, Brisbane, CA
- MP 680 **Systematic Profiling Histone Lysine Glycerylation with Chemical Proteomics Analysis**; Yi-Cheng Sin¹; Yue Chen¹; ¹University of Minnesota, Minneapolis, MN
- MP 681 **Emerging role of legumain in innate immune response – potential link to anti-inflammatory effects**; Robert Vidmar¹; Matej Vizovišek²; Tilen Sever²; Matej Kolarič²; Petra Matjan Štefin²; Georgy Mikhaylov²; Andreja Kozak²; Thomas Reinheckel³; Boris Turk²; Marko Fonovič²; ¹Jozef Stefan Institute, Ljubljana, Slovenia; ²Jozef Stefan Institute, Jamova cesta 39, Slovenia; ³Institute of Molecular Medicine, University of Freiburg, Freiburg, Germany
- MP 682 **Defining Ubiquitin Role in DNA-Protein Crosslink Repair using Mass Spectrometry**; Luke Erber¹; Natalia Tretyakova²; ¹University of Minnesota, Minneapolis, MN; ²University of Minnesota, Twin Cities, Minneapolis, MN
- MP 683 **Development of Improved Detection Methods for Proteomic Analysis of Tyrosine Sulfation**; Cayla Rose¹; Matt Davison¹; Charles Dann¹; ¹Indiana University Bloomington, Bloomington, IN
- MP 684 **LC-MS Identified Esterification of Glutamic Acid by Sorbitol in a Monoclonal Antibody Stability Assessment**; Bin Yu¹; Shannon Williams¹; Glen Young¹; ¹coherus bioscience, Camarillo, CA
- MP 685 **Boosting the sensitivity of electron-based fragmentation with cyclic ion mobility**; Dale A Cooper-Shepherd¹; Emma Marsden-Edwards¹; Darren Hewitt¹; Jason Wildgoose¹; Samantha Ippoliti¹; James I. Langridge¹; ¹Waters Corporation, Wilmslow, United Kingdom
- MP 686 **In-depth and integrated proteomics of thiol oxidation and phosphorylation for a holistic view of cell signaling**; Austin Gluth^{1,2}; Xiaolu Li¹; Matthew J Gaffrey¹; Marina A Gritsenko¹; Kiall Francis G Suazo³; Chia-Feng Tsai¹; Mowei Zhou⁴; Song Feng¹; Amy C Sims⁵; Wei-Jun Qian¹; Tong Zhang¹; ¹Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; ²Department of Biological Systems Engineering, Washington State University, Richland, WA; ³Chemical Biology, Pacific Northwest National Lab, Richland, WA; ⁴Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; ⁵Chemical and Biological Signatures Division, Pacific Northwest National Lab, Richland, WA
- MP 687 **Inhibition of Deamidation and Oxidation Artifacts in LC-MS Multi-attribute Method (MAM)**; Pingli Wei¹; Gordon Nicol¹; Ping Jiang¹; Jie Ding¹; ¹PPD Inc, Madison, WI

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- MP 688 **Chemical proteomics and data independent acquisition enable drug target identification in Mycobacterium tuberculosis**; Dietrich Mostert¹; Josef Braun²; Stephan Sieber¹; ¹Technical University of Munich, Munich, Germany; ²Technical, Munich, Germany
- MP 689 **A Proteomic Investigation of Clarithromycin Resistance and Susceptibility in Mycobacterium abscessus and Mycobacterium massiliense**; Sung Hwan Yoon¹; Ebru Selen²; Eva Le Run²; Shamira Shallom²; Adrian Zelazny²; Aleksandra Nita-Lazar¹; ¹NIH/NIAID, Bethesda, MD; ²NIH/Clinical Center, Bethesda, MD
- MP 690 **Assessment of mRNA vaccine stability by evaluating protein expression of SARS-CoV-2 spike protein with isotope dilution mass spectrometry**; Paul Branham¹; Yulanda M. Williamson²; Hans C. Cooper²; Fabio N. Najjar¹; John R Barr²; Tracie L. Williams²; ¹Oak Ridge Institute for Science and Education, Atlanta, GA; ²National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, GA
- MP 691 **Novel colistin resistance profiles of Acinetobacter nosocomialis clinical isolate, KAN02**; Hyoung Lee^{1,2}; Sung Ho Yun¹; Sang-Yeop Lee¹; Changkyun Edmond Park^{1,2}; Seung Il Kim¹; ¹Korea Basic Science Institute, Ochang, South Korea; ²Korea Research Institute of Bioscience and Biotechnology, Yuseong-gu, South Korea
- MP 692 **Serum Proteomics of COVID-19 Samples Analysed by Liquid Chromatography and SELECT SERIESTM Cyclic Ion Mobility Mass Spectrometer**; Aishath Shaufa Shareef¹; Eleanor Matthews¹; Leroy B. Martin III²; Matthew E. Daly^{1,3}; Christopher J. Hughes³; Lee Gethings^{1,3,4}; Robert Plumb²; Simpson Angela¹; Timothy Felton¹; Fowler Stephen¹; Clare Mills^{1,4}; ¹The University of Manchester NHS Foundation Trust, Manchester, United Kingdom; ²Waters, Milford, MA; ³Waters Corporation, Wilmslow, United Kingdom; ⁴The University of Surrey, Guildford, United Kingdom
- MP 693 **Mass Spectrometry Reveals How Iron and Zinc Accumulation Pathways Promote Azole Resistance in a Clinical Isolate of Aspergillus fumigatus**; Catalina Avendaño¹; Margarita Semis¹; Daniel Röth¹; Rose S. Atukunda¹; Karine Bagramyan¹; Lotus Lofgren²; Sanjeet Dadwal¹; Jason E. Stajich²; Markus Kalkum¹; ¹City of hope, Duarte, CA; ²University of California, Riverside, Riverside, CA
- MP 694 **Malaria's Plasmodium vivax Invasion Receptors? Mass Spectrometric Comparison of the Membrane Proteomes of Erythrocytes, Reticulocytes, JK-1, and BEL-A cells**; Jessica S Molina¹; Daniel Röth¹; Manuel Alfonso Patarroyo^{2,3}; Markus Kalkum¹; ¹City of hope, Duarte, CA; ²Fundación Instituto de Inmunología de Colombia, Bogotá, Colombia; ³Faculty of Medicine, Universidad Nacional de Colombia, Bogotá, Colombia
- MP 695 **A novel immunoproteomic approach to MHC class I-restricted peptide discovery for influenza CD8+ T cell adaptive vaccine development**; Richard Brase¹; Sutopa Dwivedi¹; Hager Mohamed¹; Aykan Karabudak¹; Patrick Romano¹; Brian Pfister¹; Xiaofang Huang¹; ¹Emergex USA, Doylestown, PA
- MP 696 **Novel gene identification in the influenza virus infection model using multi-omics approach, reveals potential CD8+ T-cell adaptive vaccine candidates**; Sutopa Dwivedi¹; Richard Brase¹; Hager Mohamed¹; Aykan Karabudak¹; Patrick Romano¹; Brian Pfister¹; Xiaofang Huang¹; ¹Emergex USA, Doylestown, PA
- MP 697 **Borrelia PeptideAtlas: A proteome resource for the Lyme disease community**; Helisa Wipfel¹; Jaipal P Reddy¹; Zhi Sun¹; David H Baxter¹; David D. Shteynberg¹; Melissa Caimano²; Robert L. Moritz¹; ¹Institute for Systems Biology, Seattle, WA; ²University of Connecticut School of Medicine, Farmington, CT
- MP 698 **Fast and sensitive detection of Urinary Tract Infections through SRM monitoring of machine learning defined peptide signatures**; Clarisse Gotti¹; Florence Roux-Dalvai¹; Antoine Lacombe-Rastoll¹; Charles Maxey²; Cristina Jacob²; Ève Bérubé³; Maurice Boissinot³; Michel N. Bergeron³; Neloni Wijeratne²; Claudia Martins²; Arnaud Droit¹; ¹Proteomics Platform and Computational Biology laboratory, CHU de Québec Université Laval Research Centre, Québec, QC; ²Thermo Fisher Scientific, San Jose, CA; ³Infectiology Research Centre, CHU de Québec Université Laval Research Center, Québec, QC
- MP 699 **Lipidomic and proteomic analysis of the ferroptosis-like killing of S. aureus by arachidonic acid**; Rutan Zhang¹; Ismael A. Barreras Beltran¹; Quynh Do¹; Brian J. Werth¹; Libin Xu¹; ¹University of Washington, Seattle, WA
- MP 700 **In-containment Orbitrap mass spectrometry analysis of proteomic changes during SARS-CoV-2 infection in a Syrian golden hamster (Mesocricetus auratus) model**; Kayla Adcock¹; Daniel G. Mead¹; Franklin E. Leach III¹; ¹University of Georgia, Athens, GA
- MP 701 **DDA- and DIA-PASEF profiling of cross-kingdom infections reveals new mechanisms driving disease**; Brianna Ball¹; Arjun Sukumaran¹; Jonathan R Krieger²; Jennifer Geddes-McAlister¹; ¹University of Guelph, GUELPH, ON; ²Bruker Ltd., Milton, ON
- MP 702 **Top-Down Proteomics Platform Enabled by Photocleavable Surfactant Azo for the Comprehensive Characterization of Endogenous Phospholamban**; Holden T Rogers¹; David S Roberts¹; Eli J Larson¹; Jake A Melby¹; Kalina J Rossler²; Austin V Carr¹; Kyle A Brown^{1,3}; Ying Ge^{1,2,4}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²Department of Cell and Regenerative Biology, University of Wisconsin - Madison, Madison, WI; ³Department of Surgery, University of Wisconsin-Madison, Madison, WI; ⁴Human Proteomics Program, University of Wisconsin - Madison, Madison, WI
- MP 703 **Comprehensive Characterization of Protein Kinases by Native Top-Down Mass Spectrometry**; Hsin-Ju Chan¹; Brad H. Li²; Boris Krichel²; David S. Roberts¹; Ying Ge^{1,2,3}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; ³Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI
- MP 704 **Systematic optimization of electron activated dissociation for top-down targeted protein sequencing**; Jason Causon¹; Ihor Batruch¹; ¹SCIEX, Concord, ON
- MP 705 **Identifying and characterizing heme-acquisition mechanisms in C. diphtheriae using a combination of bottom-up and native top-down proteomics**; Andrew K Goring¹; Robert T Clubb¹; Rachel R. Ogorzalek Loo¹; Joseph A. Loo¹; ¹University of California, Los Angeles, Los Angeles, CA
- MP 706 **An integrated structural proteomics pipeline to study membrane proteins in Arabidopsis thaliana tissues**; Stephanie Thibert¹; Jesse Wilson¹; Vimal Balasubramanian¹; Deseree Reid²; John Melchior^{3,4}; Kim Hixson⁵; Tanya Winkler¹; Roza Wojcik²; Aivett Bilbao¹; Jennifer E. Kyle³; Mowei Zhou¹; ¹Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; ²National Security Directorate, Pacific Northwest National Laboratory, Richland, Washington; ³Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; ⁴Department of Pathology and Laboratory Medicine, University of Cincinnati Medical School, Cincinnati, Ohio; ⁵Physical and Computational Sciences Division, Pacific Northwest National Laboratory, Richland, Washington
- MP 707 **Enhanced Top-Down Mass Spectrometry Performance with a Hybrid Quadrupole-Multireflecting Time-of-Flight System**; Brad J. Williams¹; Dale A. Cooper-Shepherd²; Barbara J. Sullivan³; James I. Langridge²; Joseph A. Loo⁴; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Wilmslow, United Kingdom; ³Waters Corporation, Milford,

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- MP 708 **Capillary Zone Electrophoresis-Mass Spectrometry Reveals Histone Modification Patterns during Zebrafish Embryonic Development;** Fei Fang¹; Qianyi Wang¹; Liangliang Sun¹; ¹Michigan State University, East Lansing, MI
- MP 709 **Evaluation of Proteoform Identification by Top-Down Data-Dependent and Data-Independent Acquisition Mass Spectrometry;** Abdul Rehman Basharat¹; Tian Xu²; Yong Zang³; Liangliang Sun²; Xiaowen Liu⁴; ¹Indiana University - Purdue University Indianapolis, Indianapolis, IN; ²Michigan State University, East Lansing, MI; ³Indiana University School of Medicine, Indianapolis, IN; ⁴Tulane University School of Medicine, New Orleans, LA
- MP 710 **Structural diversity of kinase complexes revealed by top-down mass spectrometry with micro-scale size exclusion chromatography;** Boris Krichel^{1,2,3}; Jake A Melby⁴; Holden T Rogers⁴; Eli J Larson⁴; Kevin M. Buck⁴; Emily A Reasoner⁴; Hsin-Ju Chan⁴; Charlotte Uetrecht^{2,3,5,6}; Ying Ge^{1,4,7}; ¹Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; ²University of Siegen, Siegen, Germany; ³CSSB, Center for Structural Systems Biology, Hamburg, Germany; ⁴Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ⁵German Electron Synchrotron DESY, Hamburg, Germany; ⁶Leibniz Institute of Virology (LIV), Hamburg, Germany; ⁷Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI
- MP 711 **Improved Dissociation Efficiency of Protein Ions within a Trapped Ion Mobility Device via Supercharging and Dynamic Control of Ion Count;** Katherine A Graham¹; Charles F Lawlor¹; Nicholas B Borotto¹; ¹University of Nevada Reno, Reno, NV
- MP 712 **Towards top-down proteomics of large proteoforms using capillary zone electrophoresis-tandem mass spectrometry;** Olivia Gordon¹; Liangliang Sun¹; ¹Michigan State University, East Lansing, MI
- MP 713 **Comprehensive Quantitative Top-Down Proteomic Profiling to Understand Mechanism of Action Of Kinase Inhibitor in Cancer Cells;** Trishika Chowdhury¹; Yanting Guo¹; Kellye A Cupp-Sutton¹; Si Wu¹; ¹University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK
- MP 714 **Improved characterization of the intact mammalian proteome >30 kDa using targeted proton transfer charge reduction (tPTCR);** Jake T Kline¹; Amal M Kamal¹; Jingjing Huang²; David Bergen²; Joseph B Greer³; Kenneth R Durbin³; Graeme C McAlister²; Vlad Zabrouskov²; Christopher Mullen²; Luca Fornelli¹; ¹University of Oklahoma, Norman, OK; ²Thermo Scientific, San Jose, CA; ³Proteinaceous, Evanston, IL
- MP 715 **GeLC-FAIMS-MS Workflow for Middle-Down Proteomics;** Nobuaki Takemori¹; Ayako Takemori¹; Philipp T. Kaulich²; Ryo Konno³; Yusuke Kawashima³; Yuto Hamazaki⁴; Ayuko Hoshino⁴; Andreas Tholey²; ¹Ehime University, Toon, Japan; ²Christian-Albrechts-Universität zu Kiel, Kiel, Germany; ³Kazusa DNA Research Institute, Kisarazu, Japan; ⁴Tokyo Institute of Technology, Yokohama, Japan
- MP 716 **Filling the gaps in peptide maps: variable-flowrate SEC top-down MS platform for discovery-stage protein characterization;** Aaron O Bailey¹; Lee K Palmer¹; Kenneth R. Durbin²; William Russell¹; ¹University of Texas Medical Branch, Galveston, TX; ²Proteinaceous, Evanston, IL
- MP 717 **In-Source Fragmentation Data Increases Proteoform Identifications in Complex Samples;** Austin Carr¹; Mark Scalf¹; John G. Pavek¹; Michael R. Shortreed¹; Lloyd M. Smith¹; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- MP 718 **Increased Dimensional Analysis of Native Proteins via Synthetic Nanopore;** Mario Rodriguez Garcia¹; John R. Yates III¹; ¹Scripps Research, La Jolla, CA
- MP 719 **Towards deep top-down protein analysis by tandem-trapped ion mobility spectrometry/mass spectrometry coupled with parallel accumulation serial fragmentation (tandem-TIMS/PASEF);** Christian Bleiholder¹; Fanny C Liu¹; Jusung Lee¹; Melvin A Park²; Mark E Ridgeway²; Alina Theisen³; Christopher A. Wootton⁴; Stephen Fried⁵; ¹Florida State University, Tallahassee, FL; ²Bruker Daltonics, Billerica, MA; ³Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ⁴Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ⁵Johns Hopkins University, Baltimore, MD
- MP 720 **MASH Native: A Unified Solution for Native Top-Down Proteomics Data Processing;** Sean J. McIlwain¹; Eli J. Larson¹; Melissa R. Pergande¹; Michelle E. Moss¹; Kalina J. Rossler¹; R. Kent Wenger¹; Boris Krichel^{1,2}; Harini Josyer¹; Jake A. Melby¹; David S Roberts¹; Kyndalanne A. Pike¹; Zhouxin Shi¹; Hsin-Ju Chan¹; Bridget Knight¹; Holden T. Rogers¹; Kyle A. Brown¹; Irene M. Ong¹; Kyowon Jeong³; Michael T. Marty⁴; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI; ²University of Siegen, Siegen, Germany; ³University of Tübingen, Tübingen, Germany; ⁴University of Arizona, Tucson, AZ
- MP 721 **Analysis of intact protein assemblies directly from living yeast colonies by native LESA mass spectrometry;** Yuying Du¹; Robin C. May¹; Helen J. Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom
- MP 722 **Proteome profiling of rat brain cortical changes during the early postnatal brain development using a surfactant-free protocol and label-free quantitation;** Witold M Winnik¹; William Padgett¹; Emily M Pitzer¹; David W Herr¹; ¹US EPA, Research Triangle Park, NC
- MP 723 **Absolute Quantitation of Peptides and Proteins After Derivatization by Coulometric Mass Spectrometry;** Praneeth Ivan Joel Fnu¹; Md Tanim-AI-Hassan¹; Yongling Ai¹; Hao Chen¹; ¹New Jersey Institute of Technology, Newark, NJ
- MP 724 **APEX Labeling and LC-MS/MS Analysis for Exploring the Proximity Proteome of YY1;** Zhongwen Cao¹; Yenyu Yang¹; Yinsheng Wang¹; ¹900 University Ave, Riverside, CA 92521, Moreno Valley, CA
- MP 725 **Application of Mass Spectrometry-Based Methods to Define the Cell-Surface Proteome of Murine Intestinal Organoids;** Dylan Z Dieters-Castator¹; Paolo Manzanillo¹; Daryl Bulloch¹; Han-Yin Yang¹; David Chow¹; Aman Makaju²; Bradford Gibson¹; ¹Amgen, South San Francisco, CA; ²Amgen, Thousand Oaks, CA
- MP 726 **Solution-stabilized TMT & TMTpro reagents in 96-well plates for high-throughput sample processing;** Dustin Frost¹; Ryan Bomgarden¹; ¹Thermo Fisher Scientific, Rockford, IL
- MP 727 **14-plex DeAla Isobaric Tags for High-Throughput Quantitative Proteomics;** Peng-Kai Liu¹; Ting-Jia Gu²; Danqing Wang³; Lingjun Li^{1,2,3}; ¹Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ³Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- MP 728 **Deciphering phytocannabinoid pharmacological effects using C. elegans, proteomics and bioinformatics.;** Fatma Boujenoui¹; Jennifer Ben Salem¹; Bruno Nkambeu¹; Francis Beaudry¹; ¹Universite de Montreal, St-Hyacinthe, QC
- MP 729 **Determination of vanilloid targets in Caenorhabditis elegans using Thermal proteome profiling;** Bruno Nkambeu¹; Jennifer Ben Salem¹; Francis Beaudry¹; ¹Universite de Montreal, St-Hyacinthe, QC
- MP 730 **Systematic investigation of the N-terminal effect on protein stability;** Zeyu Wang¹; Senhan Xu¹; Kejun Yin¹; Xing Xu¹; Ronghu Wu¹; ¹School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA

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- MP 731 **A Benchmarking Workflow for High-Throughput DIA Label-Free Quantification using a Novel High-Resolution Accurate Mass Platform;** [Anna V. Pashkova](#)¹; Julia Kraegenbring¹; Pedro Navarro¹; Tabiwang N. Arrey¹; Eduard Denisov¹; Hamish Stewart¹; Jeff Op De Beeck²; Nicolaie Eugen Damoc¹; ¹*Thermo Fisher Scientific, Bremen, Germany*; ²*Thermo Fisher Scientific, Ghent, Belgium*
- MP 732 **A Comparative Spatial Quantitative Proteomics Analysis of LBD Human Brain;** [Ju Wang](#)¹; Huan Sun¹; Zhiping Wu¹; Junmin Peng¹; ¹*St. Jude Children Research Hospital, Memphis*
- MP 733 **Proteomic and Phosphoproteomic Investigation of Neural Stem Cell to Oligodendrocyte Precursor Cell Differentiation Reveals Phosphorylation-Dependent Processing of Dclk1;** [Robert Hardt](#)¹; Alireza Deghghani¹; Carmen Schoor¹; Markus Gödderz¹; Nur Cengiz¹; Shiva Ahmadi¹; Ramesh Sharma¹; Karin Schork^{2,3}; Martin Eisenbacher^{2,3}; Volkmar Giesemann¹; Dominic Winter¹; ¹*Institute for Biochemistry and Molecular Biology, Medical Faculty, Rheinische Friedrich-Wilhelms-University of Bonn, Bonn, Germany*; ²*Medizinisches Proteom-Center, Medical Faculty, Ruhr-University Bochum, Bochum, Germany*; ³*Medical Proteome Analysis, Center for Protein Diagnostics, Ruhr-University Bochum, Bochum, Germany*
- MP 734 **Quantitative spatial proteomics combined with lipidomic analysis of human hippocampus using laser capture microdissected cells from MALDI-imaged tissue sections;** [Lauren R. DeVine](#)¹; Caitlin M. Tressler¹; Rahul A. Bharadwaj²; Kristine Glunde¹; Daniel Weinberger²; Robert N. Cole¹; ¹*Johns Hopkins School of Medicine, Baltimore, MD*; ²*Lieber Institute for Brain Development, Baltimore, MD*
- MP 735 **Ultra-high-resolution MS1-quantification combined with deconvolution of chimeric MS/MS spectra enables in-depth quantitative proteomics and application in high-quality spatial proteomics;** [Shuo Qian](#)¹; Shichen Shen²; Shihan Huo²; Sailee Rasam²; Min Ma¹; Jun Qu^{1,2}; ¹*Roswell Park Comprehensive Cancer Center, Buffalo, NY*; ²*University at Buffalo, Buffalo, NY*
- MP 736 **Spatiotemporally Resolved Notch Interactions on its Path from Membrane to Nucleus;** [Marian Kalocsay](#)¹; Alexandre P Martin²; Gary Bradshaw²; Robyn J Eisert²; Stephen C Blacklow²; ¹*UT MD Anderson Cancer Center, Houston, TX*; ²*Harvard Medical School, Boston, MA*
- MP 737 **A Chemoproteomic Approach for the Quantitative Identification of Arsenic-Binding Nuclear Proteins;** [Shiyuan Guo](#)¹; Pengcheng Wang²; Yinsheng Wang²; ¹*University of California Riverside, Riverside, CA*; ²*University of California, Riverside, Riverside, CA*
- MP 738 **Quantitative Assessment of Epitranscriptomic Reader, Writer and Eraser Proteins Modulated by H4K16ac and H3K36me3;** [Jiekai Yin](#)¹; Tianyu Qi¹; Lin Li¹; Yinsheng Wang¹; ¹*University of California, Riverside, Riverside, CA*
- MP 739 **FragPipe-Analyst: an interactive and user-friendly web application for the analysis of quantitative proteomics data;** [Yi Hsiao](#)¹; Haijian Zhang²; Ginny Xiaohe Li³; Fengchao Yu³; Felipe Da Veiga Leprevost³; Ralf B Schittenhelm²; Alexey I. Nesvizhskii^{1,3}; ¹*Department of Computational Medicine and Bioinformatics, Ann Arbor, MI*; ²*Monash Proteomics & Metabolomics Facility, Department of Biochemistry and Molecular Biology, Biomedicine Discovery Institute, Monash University, Clayton, Australia*; ³*Department of Pathology, University of Michigan, Ann Arbor, MI*
- MP 740 **Targeted proteomics analysis of metabolic pathway proteins to develop and optimize Chinese Hamster Ovary (CHO) cell culture medium and feed;** [Km Shams Ud Doha](#)¹; Chengjian Tu¹; Asik Didar¹; Jaime Goldfuss¹; Scott J. Jacobia¹; Andrew M. Campbell¹; ¹*Thermo Fisher Scientific, Grand Island, NY*
- MP 741 **Benchmarking the performances of label-free protein quantitation: Data dependent acquisition (DDA) vs. data independent acquisition (DIA);** [Ling Li](#)¹; Belinda Willard¹; ¹*Cleveland Clinic, Cleveland, OH*

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

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Artificial Intelligence in MS Instrumentation and Applications.....	042-062
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Biomarkers: Quantitative Analysis II.....	088-111
Cancer Research II	112-135
Clinical Analysis II	136-166
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TP 001	Single Fiber Quantitation of Solid-Phase Microextraction Samples with Five-shot Direct Analysis; <u>G. Asher Newsome</u> ¹ ; Erin R. Birdsall ^{1,2} ; Hannah A. Lawther ¹ ; ¹ Smithsonian Museum Conservation Institute, Suitland, MD; ² Smithsonian National Museum of the American Indian, Suitland, MD
TP 002	Time-course monitoring of Hexafluorophosphate decay using Soft Ionization by Chemical Reaction In Transfer (SICRIT) ion source; <u>Motoshi Sakakura</u> ¹ ; Teruhisa Shiota ¹ ; ¹ AMR Inc., Meguro-Ku, Japan
TP 003	The Role of Ion Suppression in Secondary Electrospray Ionization-Mass Spectrometry; <u>Cedric Wuethrich</u> ¹ ; Stamatios Giannoukos ¹ ; Renato Zenobi ¹ ; ¹ ETH Zurich, Zurich, Switzerland
TP 004	Understanding of phenomena of Si deposition on the electrode in counter flow atmospheric pressure chemical ionization source; <u>Shun Kumano</u> ¹ ; Satoshi Wakita ¹ ; Hisashi Nagano ² ; Tatsuo Nojiri ² ; ¹ Research & Development Group, Hitachi Ltd., Kokubunji-Shi, Japan; ² Digital Systems & Services, Hitachi Ltd., Omika, Japan
TP 005	A new frontier of direct analysis: real-time in electron ionization detection (REI)first coupling of ambient sampling with electron ionization; <u>Adriana Ariò</u> ¹ ; Giovanna Nevola ¹ ; Giorgio Famigliani ¹ ; Pierangela Palma ^{1,2} ; Achille Cappiello ^{1,2} ; ¹ UNIVERSITY OF URBINO CARLO BO, URBINO, Italy; ² Vancouver Island University, Nanaimo, BC
TP 006	Infrared Matrix-Assisted Laser Desorption Electrospray Ionization with a Heated Electrospray Emitter; <u>Kevan T. Knizner</u> ¹ ; David C. Muddiman ¹ ; ¹ FTMS Laboratory for Human Health Research, Department of Chemistry, Raleigh, NC
TP 007	Biocompatible solid-phase microextraction pin-probe electrospray ionization-mass spectrometry system facilitates high sensitivity and ease of automation; <u>Wei Zhou</u> ¹ ; Janusz Pawliszyn ¹ ; ¹ University of Waterloo, Waterloo, ON
TP 008	Comprehensive characterization of an engineered Cas9 protein and its post-translational modifications (PTMs) by LC-MS/MS; <u>Zhichang Yang</u> ¹ ; Sahana Mollah ² ; Chao-Xuan Zhang ³ ; Alicia Powers ⁴ ; Yan Lu ³ ; ¹ SCIEX, CA, USA; ² Sciex, Brea, CA; ³ St. Jude Children's research hospital, Memphis, TN; ⁴ St. Jude Children's Research Hospital, Memphis, TN
TP 009	Contained Secondary Electrospray Ionization Mass Spectrometry: Toward High-Throughput Screening of Amines as CO2 Capture Reagents ; <u>Dmytro S Kulyk</u> ¹ ; Taghi Sahraei ¹ ; Ayesha Seth ¹ ; Abraham Kwame Badu-Tawiah ¹ ; ¹ The Ohio State University, Columbus, OH
TP 010	Single Spot (<1mm) Dewaxing and Analysis of Paraffin-Embedded Tissue sections using Liquid Microjunction Sampling Probe (LMJ-SSP) mass spectrometry (MS); <u>Haidy Metwally</u> ¹ ; Malek Hassan ¹ ; Jessie Deng ¹ ; Richard D. Oleschuk ¹ ; ¹ Queen's University, Kingston, ON
TP 011	Rapid in-line solvent switching for liquid micro-junction surface sampling probe (LMJ-SSP) based mass spectrometry detection; <u>Jian Yu</u> ¹ ; Malek Hassan ¹ ; Richard D. Oleschuk ¹ ; ¹ Queen's University, Kingston, ON
TP 012	Real-time subsurface analysis and depth profiling using a sharpened liquid micro-junction surface sampling probe (LMJ-SSP); <u>Julia McPhail</u> ¹ ; Jian Yu ¹ ; Richard D. Oleschuk ¹ ; ¹ Queen's University, Kingston, ON
TP 013	ESI from surface of spherical probe made of inert fibrous material as a tool for investigation of rude biological samples; <u>Igor Popov</u> ^{1,2} ; Mariya Shamraeva ¹ ; Ekaterina Shamarina ¹ ; Stanislav Pekov ^{2,3} ; ¹ MIPT, Dolgoprudny, Russian Federation; ² Siberian State Medical University, Tomsk, Russia; ³ Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation
TP 014	Optimization of Enclosure for Introduction of Polar Organic Modifiers to Protein Analysis in DESI-MS;

TUESDAY POSTERS

- TP 015 **James A Richardson¹; Christopher J Taylor¹; Andre Venter¹; ¹Western Michigan University, Kalamazoo, MI**
Integrating the MasSpec Pen Technology with a Time-of-Flight Mass Spectrometer for Direct Tissue Analysis; Charles A. Wolfe¹; Michael F. Keating^{1,2}; Viktor Zsellers³; Tamas Karancs³; Steven Pringle³; **Justin Wiseman⁴**; Mike Morris³; Livia S. Eberlin¹; ¹Department of Surgery, Baylor College of Medicine, Houston, Texas; ²The University of Texas at Austin, Austin, TX; ³Waters Corporation, Wilmslow, United Kingdom; ⁴MS Pen Technologies Inc., Houston, Texas
- TP 016 **High-Throughput Purification, Reduction and SEC-MS Glycoprofiling of a Therapeutic Monoclonal Antibody;** **Stephan Altmaier¹**; Uma Sreenivasan²; Kevin Ray³; ¹Merck KGaA, Darmstadt, Germany; ²MilliporeSigma, Round Rock, TX; ³MilliporeSigma, St. Louis, MO
- TP 017 **Proteomic analysis reveals insights into the mechanism of intra-CORK approach for increasing therapeutic window of immunocytokines;** **Ettore Gilardoni¹**; Domenico Ravazza¹; Giulia Rotta¹; Sheila Dakhel¹; Dario Neri^{2,3}; ¹Philochem AG, Otelfingen, Switzerland; ²ETH Zurich, Zurich, Switzerland; ³Philogen S.p.A., Sovicelle, Italy
- TP 018 **Benchmarking the hinge directed proteases FabDELLO versus FabALACTICA for LC-MS based IgG1 clonal profiling;** **Danique M.H. Van Rijswijk¹**; Albert Bondt¹; Naomi De Kat¹; Jonathan Sjögren²; Rolf Lood²; Albert J.R. Heck¹; ¹Utrecht University, Utrecht, Netherlands; ²Genovis AB, Lund, Sweden
- TP 019 **Characterization of therapeutic antibody charge variants in drug development by microfluidic native capillary electrophoresis-mass spectrometry;** **Zhijie Wu¹**; Haibo Qiu¹; Ning Li¹; ¹Regeneron Pharmaceuticals, Inc, Tarrytown, NY
- TP 020 **Coupling Ion Exchange Chromatography with Native Mass Spectrometry for Charge Heterogeneity Characterization of Monoclonal Antibodies using new generation SCX column;** **Xiaoxi Zhang¹**; Sensen Chen¹; Christof Mitterer²; Min Du³; Ken Cook⁴; ¹ThermoFisher Scientific, Shanghai, China; ²Thermo Fisher Scientific, Langerwehe, Germany; ³Thermo Fisher Scientific, Boston, MA; ⁴Thermo Fisher Scientific, Hemel Hempstead, United Kingdom
- TP 021 **Simplified sample preparation of mAbs subclasses and subunits using electrochemical reduction for inline LC-MS analysis;** **Martin Eysberg¹**; Jonathan Bones²; Ken Cook³; Tomos E. Morgan²; Jean-Pierre Chervet⁴; ¹Antec Scientific, Boston, MA 02108; ²NIBRT, Dublin, Ireland; ³Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; ⁴Antec Scientific, Alphen a/d Rijn, Netherlands
- TP 022 **An Immunoaffinity LC-MS/MS Approach for the Quantitation of Total Antibody Drug Conjugate from PYX-201 Targeting EDB Fibronectin in Human Plasma;** **Diana Adhikari¹**; Minghao Sun²; Eric Ma²; William R. Mylott Jr.²; Shawn Harriman³; Jan Pinkas³; Elizabeth Shaheen³; Feng Yin³; ¹Pyxis Oncology, Cambridge, MA; ²PPD, Richmond, VA; ³Pyxis Oncology, Cambridge
- TP 023 **Novel icIEF-based fractionation of therapeutic antibody charge variant for LC-MS characterization;** **Xiaoqing Shen¹**; Philip Chao¹; Cheng Zhou¹; Kefei Wang¹; Faidh Hana²; Zhaohui Fan²; Amr Ali²; Jian He²; Dave Ouellette²; Roland Wang¹; Jessica Dermody¹; ¹ProteinSimple, a brand of Bio-technie.com, San Jose, CA; ²AbbVie Bioresearch Center, Worcester, MA
- TP 024 **Top-down characterization of native monoclonal antibodies obtained with electron capture dissociation on Q-ToF instruments;** **Yury V. Vasil'ev^{1,2}**; Rachel Franklin^{1,2}; Michael C Hare¹; Adrian Guthals¹; Joseph S Beckman^{1,2}; ¹e-MSion, Corvallis, OR; ²Oregon State University, Corvallis
- TP 025 **Ion Mobility-Mass Spectrometry and Collision Induced Unfolding of Chemically Modified Antibody Oligomers;** Nicole A Rivera-Fuentes¹; Brandon T Ruotolo²; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan-Ann Arbor, Ann Arbor, MI
- TP 026 **Improved cation exchange chromatography of monoclonal antibody on a monodisperse particle column enables deep characterization and biosimilarity assessment;** Sara Carillo¹; Florian Fuessl¹; Silvia Millan Martin¹; **Shanhua Lin²**; Jonathan Bones^{1,3}; ¹NIBRT, Dublin, Ireland; ²Thermo Fisher Scientific, Sunnyvale, CA; ³School of Chemical and Bioprocess Engineering, University College Dublin, Dublin, Ireland
- TP 027 **A High-Resolution UHPLC-MS based method for quantifying monoclonal antibodies from human serum;** **Connor E Gould¹**; Jake Ocque²; Robin Difrancesco²; Qing Ma²; Raymond Cha²; Gene Morse²; Troy D. Wood¹; ¹Department of Chemistry, University at Buffalo, Buffalo, NY; ²Department of Pharmacy Practice School of Pharmacy and Pharmaceutical sciences, University at Buffalo, Buffalo, NY
- TP 028 **Multiplexed Bioanalysis of Various Antibody-Drug Conjugates (ADCs) in Cynomolgus Monkey Plasma with Using Immunoaffinity LC-MS/MS;** **Eric W. Ma¹**; Minghao Sun¹; William R. Mylott Jr.¹; David Roos²; ¹PPD, Richmond, VA; ²Boehringer Ingelheim, Ridgefield, CT
- TP 029 **Unambiguous Identification and Localization of Isoaspartic Acid in Therapeutic Proteins by Optimized Enzymatic Digestion and Electron Transfer Dissociation;** **Lidong He¹**; Jason L. Richardson¹; Zhongqi Zhang¹; Les Miranda¹; Suminda Hapuarachchi¹; Jun Zhang¹; Jiu-Li Song¹; ¹Amgen, Thousand Oaks, CA
- TP 030 **Polyclonal antibody epitope mapping at single amino acid resolution for pregnancy malaria vaccine design;** **Santosh A Misal¹**; Robert Morrison²; Jonathan Renn²; Yai Doritchamou²; Martin Burkhardt²; Alassane Dicko³; Patrick Duffy²; Michal Fried¹; ¹Molecular and Pathogenesis Biomarkers Section, Laboratory of Malaria Immunology and Vaccinology (LMIV), National Institute of Allergy and Infectious Diseases (NIAID), National Institutes of Health (NIH), Bethesda, MD; ²Pathogenesis and Immunity Section, Laboratory of Malaria Immunology and Vaccinology (LMIV), National Institute of Allergy and Infectious Diseases (NIAID), National Institutes of Health (NIH), Bethesda, MD; ³Malaria Research & Training Center, Faculty of Medicine, Pharmacy and Dentistry, University of Sciences Techniques and Technologies of Bamako, Bamako, Mali
- TP 031 **Orthogonal techniques for LCMS characterization of a lysine conjugated ADC;** Lucy Fernandes¹; St. John Skilton¹; Marshall Bern¹; Krisztina Radi¹; Andreas Nägeli²; **Sabrina Forni¹**; ¹Protein Metrics, LLC, Cupertino, CA; ²Genovis AB, Lund, Sweden
- TP 032 **Zero False Positives in Multi-Attribute Method New Peak Detection with a Statistics Guided Approach;** **Qinjingwen Cao¹**; John Guan¹; Delia Li¹; Jennifer Zhang¹; Riley Togashi¹; Elizabeth Johnson¹; Jia Guo¹; Peilu Liu¹; Lance Cadang¹; Monica Sadek¹; Feng Yang¹; ¹Genentech, Inc., South San Francisco, CA
- TP 033 **Targeted Determination of the Abundant Therapeutic Monoclonal Antibody Interactome in Human Plasma, Serum, and Synthetic Mimics;** **G. Reid Bishop¹**; John J. Correia¹; ¹University of Mississippi Medical Center, Jackson, MS
- TP 034 **Determination of antibody Fab glycosylation impact on antigen binding and blocking of endogenous protein interactions by SEC and intact LC-MS;** **Daniel Woodall¹**; Christy A Thomson²; Thomas M Dillon¹; Arnold McAuley¹; Pavel Bondarenko¹; ¹Amgen Inc, Thousand Oaks, CA; ²Amgen Inc., Burnaby, BC
- TP 035 **Increasing Coverage of Host Cell Proteins by FAIMS Depletion Using Low, High, and Combined Edge Retention Times;** **Craig P Dufresne;** Thermo Fisher Scientific, West Palm Beach, FL

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- TP 036 **Facilitating LC-MS Analysis of Fusion Protein Therapeutics by Enzymatic Hydrolysis of Flexible Linkers**; Andreas Naegeli¹; Magdalena Widgren-Sandberg¹; Maria Nordgren¹; Camilla Sivertsson²; John Lindsay²; Rikke Rytter¹; ¹Genovis AB, Lund, Sweden; ²Genovis Inc, Cambridge, MA
- TP 037 **Comprehensive characterization of monoclonal antibodies (mAbs) and Antibody Drug Conjugates (ADCs) on a novel high-resolution accurate mass platform**; Kristina Srzentic¹; Angela Criscuolo²; Kai Scheffler²; Nicolaie Eugen Damoc²; ¹ThermoFisher Scientific, Basel, Switzerland; ²Thermo Fisher Scientific, Bremen, Germany
- TP 038 **Super-immunity by pan-sarbecovirus nanobodies**; Yufei Xiang¹; Wei Huang²; Hejun Liu³; Zhe Sang⁴; Sham Nambulli⁵; Jérôme Tubiana^{6,7}; Paul Duprex⁵; Dina Schneidman-Duhovny⁷; Ian A. Wilson³; Derek J. Taylor²; Yi Shi⁴; ¹Icahn School of Medicine at Mount Sinai, New York, NY; ²Case Western Reserve University, Cleveland, OH; ³The Scripps Research Institute, La Jolla, CA; ⁴Icahn School of Medicine at Mt Sinai, New York, New York, United States, NY; ⁵University of Pittsburgh, Pittsburgh, PA; ⁶Tel Aviv University, Tel Aviv, Israel; ⁷The Hebrew University of Jerusalem, Jerusalem, Israel
- TP 039 **An automated MS data workflow enabling targeted, site-specific glycosylation monitoring in continuous biopharmaceutical manufacturing**; Diego Bertaccini; Merck KGaA, Corsier-sur-Vevey, Switzerland
- TP 040 **De novo sequencing of polyclonal antibodies based on mass spectrometry**; Weiwei Peng¹; Joost Snijder¹; Maartje Huijbers²; Laurent Paardekooper²; Dana L.E. Vergoossen²; ¹University Utrecht, UTRECHT, Netherlands; ²Leiden University Medical Centre LUMC, Leiden, Netherlands
- TP 041 **Delineating the epitope diversity of recombinant monoclonal antibodies isolated from Alpaca polyclonal mixture with HDX-MS**; Dominic Narang¹; Thierry Le Bihan²; Teresa Nunez De Villavicencio Diaz¹; Bin Ma¹; Jennifer Crha¹; ¹Rapid Novor Inc., Kitchener, ON; ²Rapid Novor Inc, Kitchener
- TP 042 **MALDI-TOF Mass Spectrometry with Machine Learning for High-Throughput Screening of Raw Milk for Evidence of Mastitis**; Jon Thompson¹; Savana Everhart¹; Sumon Sarkar¹; Beth Clayton²; ¹Texas Tech University, Amarillo, TX; ²Texas Dairy Herd Improvement Association, Canyon, Texas
- TP 043 **Diving deeper with depthcharge: A transformer deep learning framework for modeling mass spectrometry data**; William E Fondrie¹; Wout Bittremieux²; Melih Yilmaz³; William S Noble³; ¹Talus Bioscience, Seattle, WA; ²University of Antwerp, Antwerpen, Belgium; ³University of Washington, Seattle, WA
- TP 044 **Mapping Competitive Activity Based Protein Profiling Data to AlphaFold2 Models**; Adam L Borne¹; Yusuf Adeshina¹; Natalia Zalitznyak¹; Luca Naef¹; Zachary Carpenter¹; ¹VantAI, New York, NY
- TP 045 **GlycoNovo: Deep learning based framework for N-linked glycan DeNovo sequencing**; Qianqiu Zhang¹; Zeping Mao¹; Weiping Sun²; Xiyue Zhang²; Ngoc Hieu Tran¹; Xin Lei²; Baozhen Shan²; Ming Li¹; ¹University of Waterloo, Waterloo, ON; ²Bioinformatics Solutions Inc, Waterloo, ON
- TP 046 **Machine learning of cancer type and tissue of origin from proteomes of 1,277 human tissue samples and 975 cell lines**; Zhaoxiang Cai¹; Zainab Noor¹; Adel T Aref¹; Emma L Boys¹; Dylan Xavier¹; Natasha Lucas¹; Steven G Williams¹; Jennifer M Koh¹; Erin Sykes¹; Rebecca C Poulos¹; Peter G Hains¹; Phillip J Robinson¹; Rosemary Balleine²; Roger R Reddel¹; Qing Zhong¹; ¹ProCan@, Children's Medical Research Institute, Faculty of Medicine and Health, The University of Sydney, Westmead, Australia; ²Westmead Institute for Medical Research, Faculty of Medicine and Health, The University of Sydney, Westmead, Australia
- TP 047 **Using protein structures predicted by AlphaFold2 to understand the fragmentation of proteins from pathogenic bacteria analyzed by MALDI-TOF-TOF-MS/MS**; Jihyun Park^{1,2}; Clifton K Fagerquist¹; ¹Produce Safety & Microbiology, Western Regional Research Center, Agricultural Research Service, USDA, Albany, CA; ²Oak Ridge Institute of Science Education, Oak Ridge, TN
- TP 048 **AI-based Comprehensive Prediction of Tandem Mass Spectra of Tryptic Peptides to Generate Proteome-Scale Mass Spectral Libraries**; Joel S Lapin^{1,2}; Xinjian Yan¹; Qian Dong¹; ¹NIST, Gaithersburg, MD; ²Georgetown University, Washington Dc, DC
- TP 049 **Transfer Learning Methods Improve Deep Fragmentation Model**; Alexandros Pachos¹; Anna Susmelj¹; Oliver M Bernhardt¹; An-phi Nguyen¹; Tejas Gandhi¹; Lukas Reiter¹; ¹Biognosys AG, Zurich, Switzerland
- TP 050 **AIMsPeak: a Convolutional Neural Network-Based Model for Ground-Truth Liquid Chromatography/Mass Spectrometry Features Selection**; Hiu-Lok Ngan¹; Zongwei Cai¹; ¹Hong Kong Baptist University, Hong Kong, China
- TP 051 **Exploring the Temporal Metabolome of "Hyperfood" Kimchi with Data-Driven Trajectory Cluster Analysis**; Ali Lotfi¹; Alla Veselkova²; Alexey Melnik¹; Kirill Veselkov³; Alexander Aksenov⁴; ¹University of Connecticut, Storrs, CT; ²Intelligify Ltd., London, United Kingdom; ³Imperial College London, London, United Kingdom; ⁴University of Connecticut, Storrs, CT
- TP 052 **Applying Automated Machine Learning for Classification and Regression in Large-Scale Clinical Proteomics Datasets**; Amir Alavi¹; Harendra Guturu¹; Guhan Venkataraman¹; Jane Lange²; Matthew Chang²; Travis Moore²; Khatereh Motamedchaboki¹; Anna Halama³; Frank Schmidt³; Karsten Suhre³; Mark Flory²; Serafim Batzoglou¹; ¹Seer, Inc., Redwood City, CA; ²Oregon Health & Science University, Portland, Oregon; ³Weill Cornell Medicine - Qatar, Education City, Qatar
- TP 053 **Estimating the uncertainty of AI predictions of the Kováts retention index**; Lewis Geer¹; Douglas Slotta¹; ¹NIST, Gaithersburg, MD
- TP 054 **Transfer learning to accurately predict retention times of modified peptides with DeepLC**; Robbin Bouwmeester¹; Alireza Nameni^{1,2}; Arthur Declercq^{1,2}; Ralf Gabriels^{1,2}; Sven Degroeve^{1,2}; Lennart Martens^{1,2}; ¹VIB-UGent Center for Medical Biotechnology, Gent, Belgium; ²Department of Biomolecular Medicine, Ghent University, Ghent, Belgium
- TP 055 **iDeepLC: A deep Learning-based retention time predictor for unseen modified peptides with a novel encoding system**; Alireza Nameni^{1,2}; Robbin Bouwmeester^{1,2}; Lennart Martens^{1,2}; Sven Degroeve^{1,2}; ¹VIB-UGent Center for Medical Biotechnology, Gent, Belgium; ²Department of Biomolecular Medicine, Ghent University, Ghent, Belgium
- TP 056 **Improving Identification Confidence in Suspect Screening of Consumer Products using Machine Learning**; William D Watson¹; Kristin A Favela¹; Jake A Janssen¹; Michael J Hartnett¹; Heath A Spidle¹; Jarod N Grossman^{2,3}; Jenna Hua²; ¹Southwest Research Institute, San Antonio, TX; ²Million Marker Wellness, Inc., Berkeley, CA; ³Agilent Technologies, Santa Clara, CA
- TP 057 **Realistic in silico generation and augmentation of mass spectrometry based proteomics data using generative adversarial networks**; Vartika Tewari¹; Sunghyun Huh²; Sangtae Kim²; Olga Vitek¹; ¹Northeastern University, Boston, MA; ²Bertis R&D Division, Bertis Inc., Seongnam-si, South Korea
- TP 058 **A novel deep learning approach to reconstruct sub-micron spatial and FT-ICR spectral mass spectrometry imaging using co-registered multimodal data**; Md

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- Inzamam Ul Haque¹; Debangshu Mukherjee²; Nikolay Borodinov²; Sylwia Stopka³; Nathalie Agar^{3,4,5}; Jacob Hinkle²; Olga S. Ovchinnikova^{1,2}; ¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN; ³Brigham and Women's Hospital, Boston, MA; ⁴Harvard Medical School, Boston, MA; ⁵Dana-Farber Cancer Institute, Boston, MA
- TP 059 **Semi-supervised Metric learning for universal representation of tandem mass spectra**; Kaiyuan Liu¹; Haixu Tang¹; ¹Indiana University Bloomington, Bloomington, IN
- TP 060 **Predicting tandem mass spectra of long peptides using fully convolutional networks**; Kaiyuan Liu¹; Zhu Rui¹; Haixu Tang¹; ¹Indiana University Bloomington, Bloomington, IN
- TP 061 **Novel supervised learning algorithms for real-time optimization of mass spectrometry-based proteomics data acquisition to improve proteome and interactome coverage**; Iryna Abramchuk¹; Yun-En Chung¹; Alona Petrova¹; Christopher Adams²; Jonathan R Krieger³; Tharan Sri Kumar³; Mathieu Lavallée-Adam¹; ¹University of Ottawa, Ottawa, ON; ²Bruker Scientific LLC, San Jose, CA; ³Bruker Ltd., Milton, ON
- TP 062 **Automating GC/MS peak integration using Machine Learning Modelling for maximizing throughput, quality and enhancing consistency**; Thomas Bispham¹; Tamas King²; Winnie Chau²; Steve Prutzman¹; ¹Agilent Technologies, Cedar Creek, TX; ²Agilent Technologies, Inc, Hong Kong, Hong Kong
- TP 063 **Comparative Analysis of Protein Folding Stability-Based Profiling Methods for the Characterization of Breast Cancer**; Morgan Bailey¹; Hyejin Park¹; Michael C. Fitzgerald¹; ¹Duke University, Durham, NC
- TP 064 **Analysis of serum metabolomics characteristics of 63 acute leukemia patients by liquid chromatography-mass spectrometry**; Wang Lei; Beijing Lu Daopei Institute of Hematology, Beijing, China
- TP 065 **Identification of Lyso-Platelet Activating Factors as Central Nervous System Biomarkers for Tay-Sachs Disease**; Pamela Kell¹; Sonali Mishra¹; Toloo Taghian²; Heather L Gray-Edwards²; Daniel S Ory³; Xuntian Jiang⁴; ¹Washington University School of Medicine, Saint Louis, MO; ²University of Massachusetts Medical School, Worcester, MA; ³Casma Therapeutics, Cambridge, MA; ⁴Washington University School of Medicine, St. Louis, MO
- TP 066 **Development of a dia-PASEF based workflow for single-shot 3K global proteomics of cerebrospinal fluid amenable to high-throughput and large cohorts**; Kazunari Sasaki¹; Takeo Kamakura¹; Yuanqing Ye²; Satya Saxena²; Viswanath Devanarayan²; Pallavi Sachdev²; Kanta Horie²; ¹Eisai Co., Ltd., Tsukuba-shi, Japan; ²Eisai Inc., Nutley, NJ
- TP 067 **High-performance serum metabolic fingerprints encode breast cancer**; Yida Huang¹; Kun Qian²; ¹Shanghai Jiao Tong University, Shanghai, China; ²Shanghai Jiao Tong University, Shanghai, China
- TP 068 **Multi-omic landscapes of Nasopharyngeal Carcinoma reveal patterns associated with induction chemotherapy response**; Dongxue Wang¹; Yingqin Li²; Xianfeng Shao¹; Chunxian Ou²; Jun Ma²; Fuchu He¹; ¹Beijing Proteome Research Center, National Center for Protein Sciences, Beijing, China; ²Sun Yat-Sen University Cancer Center, Guangzhou, China
- TP 069 **Energy Depletion and Metabolic Alterations in Cellular Model of Fabry Disease**; Ryan W. Pearce¹; Jillian Kodger¹; Igor Radzikh¹; Yana I Sandlers¹; ¹Cleveland State University, Cleveland, OH
- TP 070 **Discovery proteomics identifies specific alterations in lysosomal and autophagy protein pathways in a neuronal model of proteostasis dysregulation**; Hillary Andaluz Aguilar¹; Mali Cosden¹; Lei Ma¹; Jacob Marcus¹; Robert Drolet¹; Nathan Hatcher¹; ¹Merck & Co., Inc., West Point, PA
- TP 071 **Ear-resistible: A DART-Mass Spectral Approach for the Detection of the Inner Ear Disorder "Ménière's Disease"**; Rabi A Musah¹; Allix M. Coon¹; Gavin Setzen²; ¹University at Albany-SUNY, Albany, NY; ²Albany ENT & Allergy Services, Albany, NY
- TP 072 **Development of Click Chemistry-based Affinity Purification for Sequencing (Click-seq) and Analysis of Global Interactions of Estrogen with Chromatin Molecules**; Quynh-Trang Do¹; Husam Kafeenah¹; Shu-Hui Chen¹; ¹National Cheng Kung University, Tainan, Taiwan
- TP 073 **Determination of gangliosides in urine of patients suffering from diabetic kidney disease by high resolution tandem mass spectrometry**; Raluca Ica¹; Anca Suteanu-Simulescu²; Mirela Sarbu¹; Ligia Petrica²; Alina D. Zamfir^{1,3}; ¹Department of Condensed Matter, National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; ²Department of Internal Medicine II, Division of Nephrology, "Victor Babes" University of Medicine and Pharmacy, Timisoara, Romania; ³Department of Technical and Natural Sciences, "Aurel Vlaicu" University of Arad, Arad, Romania
- TP 074 **Deep plasma proteome profiling for biomarker discovery in nonalcoholic fatty liver disease (NAFLD) patients**; Annabelle Hoegl¹; Marie Louise Nautrup Therkelsen¹; Mikkel Parsberg Werge²; Elias Badal Rashou²; Mira Thing²; Liv Eline Bjørge Hetland²; Anders Ellekær Junker²; Reza Serizawa³; Mogens Vyberg^{3,4}; Christian Toft Madsen¹; Elisabeth Douglas Galsgaard¹; Lise Lotte Gluud^{2,5}; Mads Grønberg¹; ¹Research & Early Development, Novo Nordisk A/S, Maaloev, Denmark; ²Gastro Unit, Copenhagen University Hospital, Hvidovre, Denmark; ³Department of Pathology, Copenhagen University Hospital Hvidovre, Hvidovre, Denmark; ⁴Center for RNA medicine, Aalborg University Copenhagen, Copenhagen, Denmark; ⁵Department of Clinical Medicine, University of Copenhagen, Copenhagen, Denmark
- TP 075 **Non target TOF-analysis of oxidation products of aromatic amino acids with chlorine dioxide as potential marker of cell degradation**; Ferdinand Max Wächter¹; Hendrik Kersten¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal, Germany
- TP 076 **Untargeted, deep plasma proteomics and metabolomics analysis in ΔCLN3 porcine model enabling biomarker discovery and mechanistic insights into Batten disease**; Brittany Lee¹; Christine Neville²; Ting Huang¹; Mitchell Rechtzigel³; Alex Rosa Campos⁴; Khatereh Motamedchaboki¹; Daniel Hornburg¹; Jill Weimer^{2,3}; Jon Brudvig^{2,3}; ¹Seer, Inc., Redwood City, CA; ²Amicus Therapeutics, Philadelphia, Pennsylvania; ³Pediatrics and Rare Disease Group, Sanford Research, Sioux Falls, South Dakota; ⁴Sanford Burnham Prebys, San Diego, California
- TP 077 **Proteiform Detection in Deep Plasma Proteomics through Peptide Expression Correlation**; Yingxiang Huang¹; Jian Wang¹; Alexey Stukalov¹; Ting Huang¹; Margaret Donovan¹; Daniel Hornburg¹; Asim Siddiqui¹; Anna Halama^{2,3}; Frank Schmidt^{4,5}; Karsten Suhre^{2,3}; Serafim Batzoglou¹; ¹Seer Inc., Redwood City, CA; ²Bioinformatics Core, Weill Cornell Medicine-Qatar, Education City, Qatar; ³Department of Biophysics and Physiology, Weill Cornell Medicine, New York, NY; ⁴Proteomics Core, Weill Cornell Medicine-Qatar, Education City, Qatar; ⁵Department of Biochemistry, Weill Cornell Medicine, New York, NY
- TP 078 **Untargeted metabolomics reveals predictive biomarkers for Type 2 diabetes mellitus in the Indian population**; Sneha A Rana¹; Pramod P Wangikar^{1,2}; Vivek Mishra^{1,2}; Bhushan Burkul²; Prajval Nakrani²; Rakesh Kumar Sahay³; Lakshman Kumar³; ¹Indian Institute of Technology Bombay, Mumbai, India; ²Clarity Bio Systems

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- India Pvt Ltd, Pune, India; ³osmania medical college, Hyderabad, India
- TP 079 **Very large-scale cerebrospinal fluid proteomics for biomarker discovery in multiple sclerosis;** Jakob Bader¹; Christine Makarov²; Sabrina Richter³; Friederike Held²; Patricia Skowronek⁴; Maximilian Strauss⁵; Constantin Ammar⁴; Marvin Thielert⁴; Wen-Feng Zeng⁴; Isabell Bludau⁴; Benjamin Schubert³; Fabian Theis³; Christiane Gasperi²; Bernhard Hemmer²; Matthias Mann¹; ¹Department of Proteomics, Max Planck Institute of Biochemistry, Martinsried, Germany; ²Clinical Neuroimmunology Unit, University Hospital rechts der Isar, Technical University Munich, Munich, Germany; ³Institute of Computational Biology, Helmholtz center Munich, Neuherberg, Germany; ⁴Department of Proteomics, Max Planck Institute of Biochemistry, Martinsried, Munich, Germany; ⁵NNF Center for Protein Research, University of Copenhagen, Copenhagen, Denmark
- TP 080 **diaPASEF-based comparative proteomics analysis of blood-derived exosomes from drug naïve Parkinson's disease (PD) patients in two independent patient cohorts;** Laura F Dagley^{1,2}; Ai Huey Tan³; Samantha J Emery-Corbin^{1,2}; Jumana M Yousef^{1,2}; Ahmed Mohamed^{2,4}; Andrew Evans⁵; Seong-Seng Tan⁶; Shen-Yang Lim³; Han-Joon Kim⁷; Andrew I Webb^{1,2}; ¹Advanced Technology and Biology Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Australia; ²Department of Medical Biology, University of Melbourne, Parkville, Australia; ³Faculty of Medicine, University of Malaya, Kuala Lumpur, Malaysia; ⁴Bioinformatics Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Australia; ⁵Movement Disorders Service, Department of Neurology, Royal Melbourne Hospital, Parkville, Australia; ⁶Department of Medicine, Royal Melbourne Hospital, Parkville, Australia; ⁷Department of Neurology and Movement Disorder Center, Seoul National University Hospital, Jongno-gu, South Korea
- TP 081 **Interferon-γ modulates tissue metabolic response during Chagas disease;** Azadeh Nasuhidehnavi¹; Mahbobeh Lesani²; Jarrod A Roach¹; Monica Ness¹; Micah D'Armand De Chateauviex¹; Laura-Isobel McCall^{1,2}; ¹University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; ²University of Oklahoma, Department of Microbiology and Plant Biology, Norman, OK
- TP 082 **A machine learning approach of metabolomic, clinical and comorbidity data to predict COVID-19 severity and hospitalization duration;** Georgia Charkoftaki¹; Reza Aalizadeh²; Alvaro Santos-Neto³; Wan Ying Tan⁴; Emily A. Davidson⁴; Varvara Nikolopoulou²; Yewei Wang⁴; Brian Thompson⁴; Tristan Furnary⁵; Ying Chen⁴; Elsie Wunder⁴; Andreas Coppi¹; Wade Schulz¹; Akiko Iwasaki^{1,6}; Richard W. Pierce¹; Charles S. Dela Cruz¹; Gary V. Desir¹; Naftali Kaminski¹; Shelli Farhadian¹; Kirill Veselkov^{4,7}; Rupak Datta¹; Melissa Campbell⁸; Nikolaos S. Thomaidis²; Albert I. Ko⁴; David C. Thompson⁴; Vasilis Vasiliou⁴; ¹Yale University, New Haven, CT; ²National and Kapodistrian University of Athens, Athens, Greece; ³University of São Paulo, São Carlos, Brazil; ⁴Yale School of Public Health, New Haven, CT; ⁵Harvard Medical School, Boston, MA; ⁶Howard Hughes Medical Institute, Chevy Chase, MD; ⁷Imperial College, London, London, United Kingdom; ⁸Duke University, Durham, NC
- TP 083 **Peptidomic characterization of protease activity and biomarker discovery of COPD pathogenesis associated with HIV in clinical BALF samples;** Monica E. Kruk^{1,2}; Danielle Weise¹; Sarah Samorodnitsky³; Carmen Martin-Alonso⁴; Erick Lock³; Subina Mehta²; Pratik D Jagtap²; Chris Wendt^{1,5}; Timothy J Griffin²; ¹Department of Medicine, University of Minnesota, Minneapolis, MN; ²Biochemistry, Mol. Biology and Biophysics, University of Minnesota, Minneapolis, MN; ³Division of Statistics, School of Public Health, University of Minnesota, Minneapolis, MN; ⁴Harvard-MIT Division of Health Sciences and Technology, MIT, Cambridge, Massachusetts; ⁵Minneapolis Veterans Affairs Health Care System, Minneapolis, MN
- TP 084 **Integrated workflows for mass-spectrometry based profiling of cancer cell derived extracellular vesicles in biofluids and tissues;** Jody Vykoukal¹; Taketo Kato²; Hiroyuki Katayama¹; Allison Stewart¹; Ehsan Irajizad¹; Yining Cai¹; Fuchung Hsiao¹; Jennifer B Dennison¹; Edwin J Ostrin¹; Hai T Tran¹; Carl M Gay¹; Lauren A Byers¹; Johannes Fahrman¹; Samir M Hanash¹; ¹The University of Texas MD Anderson Cancer Center, Houston, TX; ²Nagoya University, Nagoya, Japan
- TP 085 **Proteomics identification of a potential biomarker of the malnutrition associated Konzo disease in human blood plasma samples;** Victor Fourcassié¹; Matthew S. Bramble²; Florence Roux-Dalvai¹; Neerja Vashist³; Dieudonné Mumba Ngoyi⁴; Desiré Tshala-Katumbay⁴; Éric Vilain⁵; Arnaud Droit^{1,6}; ¹Proteomics platform, CHU de Québec - Université Laval Research Center, Quebec City, Québec; ²Center for Genetic Medicine Research, Children's Research Institute, Children's National Hospital, Washington, DC USA, Washington, DC; ³Center for Genetic Medicine Research, Children's Research Institute, Children's National Hospital, Washington, DC; ⁴National Institute of Biomedical Research, Kinshasa, The Democratic Republic Of Congo; ⁵Department of Genomics and Precision Medicine, The George Washington University School of Medicine and Health Sciences, Washington, DC; ⁶Computational Biology Laboratory, CHU de Québec - Université Laval Research Center, Quebec, Quebec
- TP 086 **Application of Proton Induced X-ray Emission (PIXE) spectroscopy for quantifying biological markers;** Gary A Glass¹; Todd A. Byers²; Darshpreet Kaur Saini¹; Charles T. Bowen¹; Bibhudutta Rout¹; ¹University of North Texas, Denton, TX; ²University of North Texas, Denton, Texas
- TP 087 **Dual-column ZENO-TOF System to Achieve Robust and High-Quality Plasma Proteomics;** Yi (jimmy) Zeng¹; Hao Qian¹; Mark Marispini¹; Jessica Chan¹; Megan Mora¹; Robert Zawada¹; Philip Ma¹; Bruce Wilcox¹; ¹PrognomiQ Inc, San Mateo, CA
- TP 088 **Peptidomics analysis reveals changes in small urinary peptides in patients with interstitial cystitis/bladder pain syndrome;** Md Shadman Ridwan Abid¹; Haowen Qiu^{2,3}; Bridget A. Tripp³; Aline de Lima Leite³; Heidi E. Roth¹; Jiri Adamec⁴; Robert Powers^{1,3,5}; James W. Checco^{1,3}; ¹Department of Chemistry, University of Nebraska-Lincoln, LINCOLN, NE; ²Center for Biotechnology, University of Nebraska-Lincoln, LINCOLN, NE; ³The Nebraska Center for Integrated Biomolecular Communication (NCIBC), University of Nebraska-Lincoln, LINCOLN, NE; ⁴Department of Biochemistry, University of Nebraska-Lincoln, LINCOLN, NE; ⁵Redox Biology Center, University of Nebraska-Lincoln, LINCOLN, NE
- TP 089 **2D LC-MS/MS with Direct Digestion to Enhance Quantitation of Monkey Serum hDUA in the Presence of ADA and Endogenous Enzyme;** Wenchu Yang¹; Drew Tietz²; Jiang Wu²; Sarah Yuan²; John Chen¹; Chengjie Ji¹; ¹NovaBioAssays, Woburn, MA; ²Sigilon Therapeutics, Cambridge, MA
- TP 090 **Development of Liquid Chromatography – Mass Spectrometry-Based Targetted Metabolomic Assays To Screen For Heart Failure and other Chronic diseases;** Leroy S Pakkiri¹; Lik Hang Wu²; Eugene Goh²; Poh Leong Lim²; A. Mark Richards^{2,3,4}; Chester L. Drum^{2,3,5}; ¹National university of Singapore, Singapore, Singapore; ²National University of Singapore, Singapore, Singapore; ³cardiovascular research institute, Singapore, Singapore; ⁴Christchurch heart institute, Univ. of Otago, Christchurch central city, New Zealand; ⁵national university hospital, Singapore
- TP 091 **A Universal Surrogate Matrix Assay for Urea Analysis in Biological Matrix to Support Clinical Pharmacokinetic Studies of Respiratory Diseases;** Yang

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- Tang¹; Micheal Van Parys²; Xiaorong Liang¹; Brian Dean¹; Liuxi Chen¹; ¹Genentech Inc., South San Francisco, CA; ²Labcorp, Madison, WI
- TP 092 **A multiplexed mass spectrometric assay of 42 biomarkers for high-throughput screening obesity-related clinical samples**; Taitu Lin¹; Panshak Dakup¹; Athena A. Schepmoes¹; Thomas L. Fillmore¹; Adam C. Swensen¹; Tong Zhang¹; James P. Delany²; Bret H. Goodpaster²; Jie Pu³; Tujin Shi¹; Jun Qu³; Wei-Jun Qian¹; ¹PNNL, Richland, WA; ²AdventHealth, Orlando, FL; ³University at Buffalo, Buffalo, NY
- TP 093 **A Multi-Omics Strategy to Develop and Optimize Cell Culture Media in Fed-Batch Cultivation of CHO-S, DG44, and CHO-K1 GS cells**; Chengjian Tu¹; Vyncent Nguyen²; Km Shams Ud Doha²; Alex Abreu¹; Sarah Baron¹; Didar Asik²; Scott J. Jacobia¹; Andrew M. Campbell¹; ¹Thermo Fisher Scientific, Grand Island, NY; ²Thermo Fisher Scientific, Buffalo, NY
- TP 094 **Assessment of a 60-biomarker health surveillance panel (HSP) on whole blood from remote sampling devices by LC/MRM-MS and DIA-MS analysis**; Stephen A. Whelan¹; Nathan Hendricks¹; Zachary L. Dwight¹; Qin Fu²; Annie Moradian¹; Jennifer E. Van Eyk²; Susan M. Mockus¹; ¹Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA; ²Smit Heart Institute, Advanced Clinical Biosystems Research Institute, Cedars-Sinai Medical Center, Los Angeles, California
- TP 095 **Quantitative metabolomics and lipidomics of more than 1,400 biomarkers using cloud-based workflow management software with machine learning peak integration algorithm**; Gregor Ömer¹; Markus Langsdorf¹; Tuan Hai Pham¹; Cornelia Röhring¹; Therese Koal¹; ¹biocrates life sciences ag, Innsbruck, Austria
- TP 096 **A novel quantification method for RPE phagocytosis using a VLC-PUFA-based strategy**; Fangyuan Gao; UC Irvine, Irvine 92617, CA
- TP 097 **Determination of Benzophenones in human Placenta from Northern Taiwan using a Solid-liquid Extraction-based UHPLC-MS/MS**; Ming-Hung Hsieh¹; Mei-Lien Chen²; Pei-Wei Wang^{2,3}; Wen-Po Cheng¹; Yu-Fang Huang^{*2}; ¹Department of Safety, Health and Environmental Engineering, National United University, Miaoli, Taiwan, Miaoli, Taiwan; ²Institute of Environmental and Occupational Health Sciences, National Yang-Ming Chiao Tung University, Taipei, Taiwan; ³Department of Pediatrics, Heping Fuyou Branch, Taipei City Hospital, Taipei, Taiwan
- TP 098 **Development of a workflow to assess gastric cancer antigenic biomarkers in circulation using ion-mobility mass spectrometry and enzyme-linked immunosorbent assays**; Rongzhang Dou¹; Hiroyuki Katayama²; Ehsan Irajizad²; Yining Cai²; Johannes Fahrman²; Jody Vykoukal²; Yihui Chen²; Ali Hussein Abdel Sater²; Edwin Ostrin²; Jaffer Ajani²; Samir Hanash²; ¹MD Anderson Cancer Center, Houston, TX; ²MD Anderson, Houston, TX
- TP 099 **LC-FAIMS/dCV-MS Method Enabled Ultra-sensitive Antibody-free Quantification of Low-abundance Biomarkers in Clinical Cohorts, with High Accuracy and Sensitivity**; Qingqing Shen¹; Jie Pu¹; Chao Xue¹; Wei-Jun Qian²; Cornelia L Boeser³; Claudia Martins³; Scott M Peterman³; Jun Qu^{1,4}; ¹University at Buffalo, Buffalo, NY; ²Pacific Northwest National Lab, richland, WA; ³ThermoFisher Scientific, San Jose, CA; ⁴New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY
- TP 100 **Molecular determination of survival motor neuron protein provides a breakthrough for gene therapy and newborn diagnostics of spinal muscular atrophy**; Michael Przybylski¹; Pascal Wiegand¹; Tamsila Khan¹; Stefan Maeser¹; Wolfgang Kleinekofort¹; Andreas Hahn²; ¹Centre for Analytical Biochemistry and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany; ²Department of Child Neurology, Giessen, Germany
- TP 101 **Quantitative Proteomics for Selectivity and Mechanism of Action Analysis of a Heterobifunctional STAT3 degrader In Vitro and In Vivo**; Yatao Shi¹; Eric Kuhn¹; Karen Yuan¹; Yogesh Chutake¹; Vaishali Dixit¹; Michele Mayo¹; Joyoti Dey¹; Bin Yang¹; Haojing Rong¹; Phillip Liu¹; Dirk M Walther¹; Chris De Savi¹; Kirti Sharma¹; ¹Kymera Therapeutics, Watertown, MA
- TP 102 **Serum N-Glycan Profiling of Patients with Narcolepsy type 1 Using LC-MS/MS**; Akeem Adeyemi Sanni¹; Md Abdul Hakim¹; Mona Goli¹; Samer El Hayek²; Farid Talih³; Bartolo Lanuzza⁴; Firas Kobeissy^{5,6}; Giuseppe Plazzi^{7,8}; Stefania Mondello⁹; Raffaele Ferri⁴; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX; ²Department of Psychiatry and Behavioral Sciences, University of Miami Miller School of Medicine, Miami, FL; ³Department of Psychiatry, Faculty of Medicine, American University of Beirut, Beirut, Lebanon; ⁴Sleep Research Centre, Department of Neurology IC, Oasi Research Institute- IRCCS, Troina, Italy; ⁵Faculty of Biochemistry and Molecular Genetics, American University of Beirut, Beirut, Lebanon, Beirut, Lebanon; ⁶Morehouse School of Medicine (MSM), Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Atlanta, Georgia; ⁷IRCCS, Istituto delle Scienze Neurologiche di Bologna, Bologna, Italy; ⁸Department of Biomedical, Metabolic and Neural Sciences, University of Modena and Reggio Emilia, Modena, Italy; ⁹Department of Biomedical and Dental Sciences and Morphofunctional Imaging, University of Messina, Messina, Italy
- TP 103 **Clinical proteomic analysis across the Alzheimer's disease continuum**; Sophia Weiner¹; Mathias Sauer¹; Nicholas Ashton¹; Pedro Rosa-Neto²; Henrik Zetterberg^{1,3}; Kaj Blennow^{1,3}; Johan Gobom^{1,3}; ¹University of Gothenburg, Gothenburg, Sweden; ²McGill University, Montreal, Québec; ³Sahlgrenska University Hospital, Gothenburg, Sweden
- TP 104 **Development of a Highly-specific LC-MS/MS based Quantitative Fecal Occult Blood Test for Canine**; Zhiyu Li¹; Hefeng Zhang¹; Siyu Liu¹; Zhiren Yu¹; Lili Xing¹; Yi Tao¹; Liang Shen¹; ¹WuXi AppTec, Shanghai, China
- TP 105 **Evaluating co-expression of tagged proteins in isolated EVs with attomole sensitivity**; Michael A Shaw¹; Dmitriy Verkhoturov²; Seonhwa Lee³; Stanislav Verkhoturov²; Michael J. Eller¹; Alexander Revzin³; Emile A. Schweikert²; ¹Department of Chemistry and Biochemistry, California State University Northridge, Northridge, California; ²Department of Chemistry, Texas A&M University, College Station, Texas; ³Department of Physiology and Biomedical Engineering, Mayo Clinic, Rochester, Minnesota
- TP 106 **High-throughput bioanalysis (BA) of serum biomarker 7aC4 using tandem LC/MS: devising an end-to-end single-vial approach in a sample-limited setting**; Soumya Kandi¹; Qin C Ji²; John P. Savaryn²; Sarah Blink Polakow²; Gary J Jenkins²; Kenneth Ruterbories²; Mary Saltarelli²; Mario Richter²; ¹Abbvie, North Chicago, IL; ²AbbVie, North Chicago, IL
- TP 107 **Integration of enhanced quantitative plasma proteomics with immunoassay for discovery of blood biomarkers for early detection of papillary thyroid carcinoma**; Hong Wang¹; Nan Jiang²; Linzhen Song²; Huanjun Ling²; Junli Gao²; Junshun Gao²; Shengpeng Ying³; Qi Chen³; ¹Hangzhou Cosmos Wisdom Mass Spectrometry Center of Zhejiang University Medical School, Hangzhou, China; ²Hangzhou Cosmos Wisdom Mass Spectrometry Center of Zhejiang University Medical School, Hangzhou, China; ³Taizhou Central Hospital, Taizhou, China
- TP 108 **Investigation of systemic inflammation induced FcRn dysregulation with sensitive LC-FAIMS-dCV-MRM**; Chao Xue¹; Qingqing Shen¹; Jie Pu¹; Yang Liu¹; Ming Zhang¹; Jun Qu^{1,2}; ¹University at Buffalo, Buffalo, NY; ²New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY

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- TP 109 **LC-MS based Discovery of Plasma Phosphopeptide Markers for Alzheimer's Disease Staging and Clinical trials;** Kyungdo Kim¹; Min-Kyung Jun¹; Se Hwan Jang¹; Byeong C. Kim²; Zee-yong Park¹; ¹*School of Life Science, Gwangju Institute of Science and Technology, Cheomdangwagi123, Buk-gu, Gwangju, South Korea;* ²*Department of Neurology, Chonnam National University Hospital, Gwangju, South Korea*
- TP 110 **NanoLC-timsTOF platform-assisted analysis of glycosylated albumin in diabetes-affected plasma and tear film;** Yanqi Tan; *University of Illinois, Urbana, IL*
- TP 111 **A Comparison of Tribrid Mass Spectrometer Architectures for Deep Blood Plasma Proteomics;** Johannes Kreuzer^{1,2}; Jingjing Huang³; Eric F Zaniewski^{1,2}; Soroush Hajizadeh^{1,2,4}; Benedikt C. Clemens^{1,2}; David Bergen³; Jesse D. Canterbury⁵; Michael W. Senko³; Graeme C McAlister³; Wilhelm Haas^{1,2}; ¹*MGH Cancer Center, Charlestown, MA;* ²*Harvard Medical School, Boston, MA;* ³*Thermo Fisher Scientific, San Jose, California;* ⁴*Broad Institute of MIT and Harvard, Cambridge, MA;* ⁵*ThermoFisher Scientific, San Jose, California*
- TP 112 **The proteome of urinary extracellular vesicles informs tumor progression in localized prostate cancer;** Amanda Khoo^{1,2}; Meinusha Govindarajan^{1,2}; Zhuyu Qiu³; Vladimir Ignatchenko²; Danny Vesprini⁴; O. John Semmes⁵; Julius O Nyalwidhe⁵; Stanley Liu^{1,4}; Paul C Boutros³; Thomas Kislinger^{1,2}; ¹*Department of Medical Biophysics, University of Toronto, Toronto, ON;* ²*Princess Margaret Cancer Centre, University Health Network, Toronto, ON;* ³*Jonsson Comprehensive Cancer Center, University of California, Los Angeles, Los Angeles, CA;* ⁴*Odette Cancer Centre, Sunnybrook Health Sciences Centre, Toronto, ON;* ⁵*Leroy T. Canoles, Jr. Cancer Research Center, Eastern Virginia Medical School, Norfolk, VA*
- TP 113 **Inoperative Margin Detection of Head and Neck Cancer with Rapid Evaporative Ionisation Mass Spectrometry;** James Anthony Higginson¹; Jasmin Werner¹; Stefania Maneta-Stavarakaki¹; Lauren Ford¹; Dani Simon¹; Yuchen Xiang¹; Jagtar Dhanda²; Zoltan Takats¹; ¹*Imperial College, London, London, United Kingdom;* ²*Brighton and Sussex Medical School, Brighton, United Kingdom*
- TP 114 **Media Component Analysis during Human Primary T Cell Culture using a Triple Quadrupole Mass Spectrometer;** Evelyn H. Wang¹; Stephen Kurzyniec¹; Erin Strom²; Tammy Jones-Lepp²; Amanda Leisgang²; Andrew Ortiz²; Jefferson Kinney²; Yoshiyuki Okamura¹; ¹*Shimadzu Scientific Instrument, Columbia, MD;* ²*University of Nevada Las Vegas, Las Vegas, NV*
- TP 115 **Studying Off-Target Effects of Small Molecule Covalent Cysteine Modifiers Using Thermal Proteome Profiling;** Andrew J Perciaccante¹; Kate Brown¹; Tapan K Maity¹; Massimiliano Bissa²; Genoveffa Franchini²; Daniel H Appella³; Ettore Appella¹; Lisa M Jenkins¹; 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 116 **Millions of cellular drug assays created by dose-resolved (phospho)proteomics reveal drug mechanism of action and decrypt post-translational modifications;** Jana Zecha¹; Florian P. Bayer¹; Nicola Berner¹; Stephan Eckert¹; Svenja Wiechmann¹; Matthew The¹; Julian Mueller¹; Karl Kramer¹; Guillaume Medard¹; Mathias Wilhelm¹; Annika Schneider¹; Maria Reinecke¹; Julia Woortman¹; Severin Lechner¹; Patroklos Samaras¹; Ludwig Lautenbacher¹; Firas Hamood¹; Polina Prokofeva¹; Stephanie Heinzlmeir¹; Benjamin Ruprecht¹; Bernhard Kuster¹; ¹*Technical University of Munich, Freising, Germany*
- TP 117 **HDAC inhibitors induce proteome remodeling of diverse lung cancer cells;** Chuwei Lin¹; Devin Schweppe¹; ¹*University of Washington, Seattle, WA*
- TP 118 **DIA proteomics method applied to probing p53-independent functions of Mdm2 and Mdmx in a human cancer cell line;** Anu Jain¹; Rafaela Muniz De Queniroz²; Jayanta K. Chakrabarty¹; Lipi Das¹; Carol Prives²; Lewis M. Brown¹; ¹*Department of Biological Sciences, Quantitative Proteomics and Metabolomics Center, Columbia University, New York, NY;* ²*Department of Biological Sciences, Columbia University, New York, NY*
- TP 119 **Parallel analysis of the proteome, histone PTMs and RNA modifications from FFPE and frozen tissue sections by MS;** Joanna K Lempiainen¹; Yixuan (axe) Xie¹; Angela C Hirbe²; Benjamin A Garcia¹; ¹*Washington University in St Louis, Department of Biochemistry and Molecular Biophysics, St Louis, MO;* ²*Washington University in St Louis, School of Medicine, Division of Oncology, St. Louis, MO*
- TP 120 **Phosphoproteomic subtyping of gastric cancer reveals dynamic transformation with chemotherapy;** Jun Adachi¹; Hirokazu Shoji²; Masahiko Aoki^{2,3}; Hidekazu Hirano²; Yuichi Abe¹; Kazufumi Honda⁴; Takeshi Tomonaga¹; Kenji Mizuguchi¹; Takaki Yoshikawa²; Narikazu Boku⁵; ¹*National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan;* ²*National Cancer Center Hospital, Tokyo, Japan;* ³*Kyoto University, Kyoto, Japan;* ⁴*Nippon Medical School, Tokyo, Japan;* ⁵*University of Tokyo, Tokyo, Japan*
- TP 121 **High-Throughput proteome profiling of in-vitro generated tumor associated macrophages reveals key signatures of immune response proteins for therapeutic applications;** Shreya Ahuja¹; Becki Dudley²; Abby J. Chiang³; Matthew S. Glover³; Lisa H Cazares³; Luca Melchiori²; Robert Wilkinson²; Dmitry Gascard³; Des Jones²; Sonja Hess³; ¹*Astrazeneca, Gaithersburg, MD;* ²*AstraZeneca, Cambridge, United Kingdom;* ³*AstraZeneca, Gaithersburg, MD*
- TP 122 **Molecular Landscapes of Breast Cancer Subtypes: Data Independent Acquisition and Identification of Potential Therapeutic Targets for Stromal Reprogramming;** Jordan B Burton¹; Deng Pan²; Joanna Bons¹; Rosemary Bai²; Chira Chen-Tanyolac²; Deborah Collyar²; Christie L Hunter³; Philippe Gascard²; Thea D Tlsty²; Birgit Schilling¹; ¹*Buck Institute for Research on Aging, Novato, CA;* ²*University of California San Francisco, San Francisco, CA;* ³*SCIEX, Redwood City, CA*
- TP 123 **Metabolic landscape identified altered arachidonic acid pathway in bladder cancer;** Mohammed Khurshidul Hassan¹; Danthasinghe Waduge Badrajee Piyaratna²; Vasanta Putluri²; Roni J. Bollag³; Martha K Terris³; Leomar Y Ballester⁴; Yair Lotan⁵; Cristian Coarfa²; Nagireddy Putluri²; ¹*Baylor College of Medicine, Houston, TX;* ²*Baylor College of Medicine, Houston, Texas;* ³*Augusta university, Augusta, Georgia;* ⁴*MD Anderson, Houston, TX;* ⁵*UT Southwestern Medical Center, Dallas, Texas*
- TP 124 **The Proteomic Changes in HCT 116 Colon Cancer Spheroids During Growth;** Catherine B Edgington¹; Nicole C. Beller²; Amanda B. Hummon²; ¹*The Ohio State University, Columbus, OH;* ²*The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH*
- TP 125 **Differing Cytoplasmic Lipid Droplet Proteomes from Vehicle-Treated and Fatty Acid Synthase-Inhibited Metastatic Breast Cancer Cells Generate Novel, Testable Hypotheses;** Chaylen J Andolino^{1,2}; Kimberly K Buhman¹; Dorothy Teegarden¹; ¹*Department of Nutrition Science, Purdue University, West Lafayette, IN;* ²*Purdue Proteomics Facility, Bindley Bioscience Center, Purdue University, West Lafayette, Indiana*
- TP 126 **Identification of Celastrol as a new E3 ligase ligand for PROTAC design;** Yufeng Xiao¹; Yi Liu¹; Zongtao Lin²; Jing Pei³; Guangrong Zheng¹; Dongwen Lv^{3,4}; ¹*Department of*

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- Medicinal Chemistry, College of Pharmacy, University of Florida, Gainesville, FL; ²Department of Biochemistry and Molecular Biophysics, Washington University in St. Louis, St. Louis, MO; ³Department of Biochemistry and Structural Biology and Center for Innovative Drug Discovery, School of Medicine, University of Texas Health Science Center at San Antonio, San Antonio, TX; ⁴Mays Cancer Center, University of Texas Health Science Center at San Antonio, San Antonio, TX
- TP 127 **Determining the role of the Uncharacterized Zinc Finger Transcription Factor Associated in Lung Adenocarcinoma (LUAD);** Xingyu Liu¹; Yixuan (axe) Xie¹; Zongtao Lin¹; Benjamin A Garcia¹; ¹Washington University School of Medicine, St. Louis, MO
- TP 128 **SUMO inhibition unveils the dark immunopeptidome in acute myeloid leukemia;** Léa Christophe¹; Mirela Pascariu¹; Chantal Durette¹; Eric Bonneil¹; Joel Lanoix¹; Marie-Pierre Hardy¹; Krystel Vincent¹; Claude Perreault^{1,2}; Pierre Thibault^{1,3}; ¹Institute of Research in Immunology and Cancer, Université de Montréal, Montreal, QC; ²Department of Medicine, Université de Montréal, Montréal, Québec; ³Department of Chemistry, Université de Montréal, Montréal, Québec
- TP 129 **Metabolic Pathways of Monounsaturated Lipids Revealed by In-depth Structural Lipidomics by Mass Spectrometry;** Simin Cheng¹; Zheng Ouyang¹; Xiaoxiao Ma¹; ¹Tsinghua University, Beijing, China
- TP 130 **Investigating Lipid Sources Contributing to Resistance to Lysosomal Autophagy Inhibition in Melanoma;** Sandra L. Harper¹; Vaibhav Jain²; Ravi K. Amaravadi²; David W. Speicher¹; Aaron R. Goldman¹; ¹The Wistar Institute, Philadelphia, PA; ²University of Pennsylvania, Philadelphia, PA
- TP 131 **Cell Viability, Purity, and Drug-Protein Interactions of Novel Gold (I) Compounds Within Various Cancer Types;** Kyle L. Wilhelm¹; Charli Worth¹; Neda Fezi¹; Shyam Pokhrel²; Ahmad Ahmad²; Mitchell Bruce²; Alice Bruce²; Joseph Taube¹; Touradj Solouki¹; ¹Baylor University, Waco, TX; ²University of Maine, Orono, ME
- TP 132 **Verification of Serum Biomarkers for High-Grade Serous Ovarian Carcinoma Recurrence by Targeted Proteomics;** Deborah Wenk¹; Shahbaz Khan¹; Vladimir Ignatchenko¹; Marcus Q. Bernardini^{2,3}; Thomas Kislinger^{1,4}; ¹Princess Margaret Cancer Centre, University Health Network, Toronto, ON; ²Division of Gynecologic Oncology, Princess Margaret Cancer Centre, University Health Network, Toronto, ON; ³Department of Obstetrics and Gynaecology, University of Toronto, Toronto, ON; ⁴Department of Medical Biophysics, University of Toronto, Toronto, ON
- TP 133 **Spatial N-Glycan Profiling of an Ovarian Cancer Mouse Model Using MALDI Mass Spectrometry Imaging;** Xin Ma¹; Soojin Park²; Thu-Huyen Pham²; Andro Botros²; Sylvia R. Yun²; Eun Young Park²; Olga Kim²; Grace Grimsley³; Jaeyeon Kim²; Richard R. Drake³; Facundo M. Fernandez¹; ¹School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; ²Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, IN; ³Department of Cell and Molecular Pharmacology and Experimental Therapeutics, Medical University of South Carolina, Charleston, SC
- TP 134 **Proteogenomic Characterization of Chemotherapy Response in Muscle Invasive Bladder Cancer;** Matthew V. Holt¹; Yongchao Dou¹; Meggie N. Young¹; Antrix Jain¹; Alexander B. Saltzman¹; Jonathan T. Lei¹; Kyle D. Drinnon¹; Sung Han Kim¹; Meenakshi Anurag¹; Bing Zhang¹; Anna Malovannaya¹; Seth P Lerner¹; ¹Baylor College of Medicine, Houston, Texas
- TP 135 **Identifications of metabolic changes upon microbiome depletion in pancreatic tumor bearing mice models;** Dominik Awad¹; Li Zhang¹; Xiaoyi Li¹; Peter Sajjakulnukit¹; Anthony Andren¹; Costas Lyssiotis¹; ¹University of Michigan-Ann Arbor, Ann Arbor, MI
- TP 136 **Multi-Omics approach to identify the molecular signature of primary non function prior to transplantation in deceased donor kidneys;** Sadr ul Shaheed¹; Fenna E.M. Van De Leemkolk²; Corinna M Snashall¹; Maria Letizia Lo Faro¹; Chris W. Sutton³; Jan H.N. Lindeman²; Rutger J. Ploeg^{1,2}; ¹Nuffield Department of Surgical Sciences, University of Oxford, Oxford, United Kingdom; ²Department of Surgery, Transplant Center Leiden University Medical Center, Netherlands; ³Institute of Cancer Therapeutics, University of Bradford, Bradford, United Kingdom
- TP 137 **Data Acquisition and Intraoperative Analysis on a mobile, battery-operated orbitrap mass spectrometer;** Michael Keating¹; Charles A. Wolfe²; Andréia de Melo Porcari²; Alexander Makarov³; Livia S. Eberlin²; ¹University of Texas at Austin, Austin, TX; ²Division of Surgical Oncology, Baylor College of Medicine, Houston, Texas; ³Thermo Fisher Scientific, Bremen, Germany
- TP 138 **Moving towards digitally-enabled clinical trials with metabolomics analysis of dried blood samples (DBS) using an at-home microsampling collection device;** Thomas P. Wyche¹; Corinne Thomas¹; Melanie Anderson²; Brad R. Evans²; Kevin P. Bateman²; Theodore R. Sana¹; ¹Merck & Co., Inc., Cambridge, MA; ²Merck & Co., Inc., West Point, PA
- TP 139 **Assisting routine diagnosis and intraoperative decisions of skin cancers using paper spray ionization miniature mass spectrometry;** Laura Min Xuan Chai¹; Hou-Chun Huang¹; Yu-Hsuan Chen¹; Jia-Fang Tsai²; Yi-Hua Liao^{2,3}; Cheng-Chih Hsu¹; ¹Department of Chemistry, National Taiwan University, Taipei City, Taiwan; ²Department of Dermatology, National Taiwan University Hospital, Taipei City, Taiwan; ³Department of Dermatology, National Taiwan University College of Medicine, Taipei City, Taiwan
- TP 140 **A Simplified Proteomics LC-MRM-MS Assay for Determination of ApoE Genotypes in Plasma Samples;** Deema O. Qasrawi¹; Rania M Khan¹; Evgeniy V. Petrotchenko¹; Manuel Montero-Odasso²; Christoph H. Borchers^{1,3,4,5}; ¹Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ²St. Joseph's Health Care, University of Western Ontario, London, ON; ³Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ⁴Division of Experimental Medicine, McGill University, Montreal, QC; ⁵Department of Pathology, McGill University, Montreal, QC
- TP 141 **Direct Quantitation of 77 Therapeutic and Clinical Toxicology Drugs in Dried Blood Spots using the Fully Automated Transcend DSX-1 System;** Jingshu Guo¹; Courtney Patterson²; Richard Gibson²; Kristine Van Natta²; Stephanie N. Samra²; ¹Thermo Fisher Scientific, Roseville, MN; ²Thermo Fisher Scientific, San Jose, CA
- TP 142 **LC-MS/MS assay to quantify the lung cancer drug Osimertinib and its Metabolites from Plasma and Microsampled Dried Blood Spots;** Bharat Venkatesh¹; Alex Yuile²; Matthew J McKay¹; Sathya Narayanan²; Helen Wheeler²; Malinda Itchins²; Nick Pavlakis²; Stephen J Clarke²; Mark P Molloy¹; ¹School of Medical Sciences, The University of Sydney, Sydney, Australia; ²Department of Medical Oncology, Royal North Shore Hospital, Sydney, Australia
- TP 143 **Simultaneous analysis of immunosuppressive drugs in whole blood samples using LC-MS/MS;** Takahiro Goda¹; Tsuyoshi Nakanishi²; Junichi Masuda¹; Natsuka Kimura³; Kenichi Aizawa³; ¹SHIMADZU Corporation, Kawasaki, Japan; ²SHIMADZU Corporation, Kyoto, Japan; ³Jichi Medical University, Shimotsuke, Japan

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- TP 144 **A new MALDI-based diagnostic method for the detection of *C. difficile* in humans;** Josef Dvorak^{1,2}; Petr Pompach^{1,3}; Jaroslav Hrabák⁴; Lukáš Fojtík^{1,2}; Petr Novák^{1,2}; ¹Department of Biochemistry, Charles University, Prague, Czech Republic; ²Institute of Microbiology of the CAS, v. v. i., Prague, Czech Republic; ³Institute of Biotechnology of the CAS, v. v. i., Prague, Czech Republic; ⁴Biomedical Center, Faculty of Medicine, Charles University, Pilsen, Czech Republic
- TP 145 **LC-MS/MS innovations geared to address the changing landscape of newborn screening;** Konstantinos Petritis¹; Samantha L Isenberg¹; C. Austin Pickens¹; Carla Cuthbert¹; ¹Centers for Disease Control and Prevention, Atlanta, GA
- TP 146 **Facile and expedited high-throughput sample preparation prior to analysis of clinically relevant free hormones from serum;** M James Ross¹; Gabriel Odugbesi¹; ¹MilliporeSigma, Bellefonte, PA
- TP 147 **Advanced patients follow-up by simultaneous quantification and structural characterization of biotherapeutic and anti-drug antibodies after administration using capillary electrophoresis-mass spectrometry;** Tessa Reinert^{1,2}; Pascal Houzé^{3,4}; Nathalie Mignet¹; Alexandre Kulus²; Matthieu Allez⁵; Yannis Nicolas Francois²; Rabah Gahoual¹; ¹Unité de Technologies Chimiques et Biologiques pour la Santé, UMR8258 CNRS, Inserm U1022, Faculty of Pharmacy, Université Paris Cité, Paris, France; ²Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, Strasbourg, France; ³Unité de Technologies Chimiques et Biologiques pour la Santé (UTCBS), CNRS UMR8258, Inserm U1022, Université de Paris, France; ⁴Laboratoire de Toxicologie Biologique, Hôpital Lariboisière, Assistance Publique – Hôpitaux de Paris (AP-HP), France; ⁵Hopital Saint-Louis, Assistance Publique – Hôpitaux de Paris (AP-HP), Paris, France
- TP 148 **Simultaneous Quantification of 13 Clinically Significant Simple and Macrocytic Trichothecenes in Human Urine Using Liquid Chromatography with Tandem Mass Spectrometry;** Claudia C Beck¹; Matthew R McIntyre¹; Dennis G Hooper¹; ¹Realtime Laboratories, Carrollton, TX
- TP 149 **Rapid identification of Methicillin-resistant Staphylococcus aureus (MRSA) and methicillin-susceptible Staphylococcus aureus (MSSA) using the MasSpec Pen Technology;** Manoj Kumar¹; Coreen L. Johnson²; Michael Keating¹; James J. Dunn²; Min Woo Sun³; Robert Tibshirani⁴; Rachel D. Downey⁵; Lindsey M. Kirkpatrick⁶; Livia S. Eberlin¹; ¹Baylor College of Medicine, Department of Surgery, Houston, Texas; ²Texas Children's Hospital, Dept. of Pathology, Houston, Texas; ³Stanford University, Departments of Biomedical Data Sciences and Statistics, Stanford, CA, Texas; ⁴Stanford University, Departments of Biomedical Data Sciences and Statistics, Stanford, CA; ⁵Dell Children's Medical Center, Austin, TX; ⁶Riley Hospital for Children, Dept. of Pediatric Infectious Diseases, Indianapolis, IN
- TP 150 **Therapeutic Drug Monitoring Using Miniature Mass spectrometer for ICU;** Jiexun Bu¹; Nan Zhang¹; Wenpeng Zhang²; Zheng Ouyang²; ¹PURSPEC Technology (Beijing) Ltd., Beijing, China; ²Department of Precision Instrument, Tsinghua University, Beijing, China
- TP 151 **Development and validation of LC-MS/MS method for the measurement of plasma aldosterone revealed interference in patient samples;** Yi Ting Tan¹; Troy Puar¹; Daryl Hee¹; ¹CHANGI GENERAL HOSPITAL, Singapore, Singapore
- TP 152 **A complete, automated end-to-end workflow for high-throughput therapeutic drug monitoring using Evosep MRM;** Angela Mc Arde¹; Magnus Huusfeldt²; Bharath Kumar Raghuraman^{1,3}; Dorte Bekker-Jensen¹; Ole Vorm¹; Nicolai Bache¹; ¹Evosep, Odense, Denmark; ²Evosep, Odense, Denmark; ³Department of Clinical Biochemistry, Biomarker Laboratory, Odense, Denmark
- TP 153 **Intelligent Reflex: A novel approach for higher throughput; improved clinical specificity and enhanced QA/QC. Application in newborn screening;** Lindsay M MacNamara¹; Samantha L Isenberg¹; Carla Cuthbert¹; Konstantinos Petritis¹; ¹CDC, Atlanta, GA
- TP 154 **Multiplex LC-MS/MS method development and validation for the simultaneous analysis of seven antibiotics from pediatric whole blood volumetric absorptive microsamples;** John Takyi-Williams¹; Ruiting Li²; Amanda Bwint³; Bo Wen²; Duxin Sun²; Marc Scheetz⁴; Kevin J. Downes³; Athena F Zuppa³; Manjunath P. Pai²; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan Ann-Arbor, Ann Arbor, MI; ³Children's hospital of Philadelphia, Philadelphia, Pennsylvania; ⁴Midwestern University, Downers Grove, Illinois
- TP 155 **Chemical biopsy acupuncture needles for direct-mass spectrometry via microfluidic open interface applied to in-vivo tissue monitoring in surgery;** Runshan W Jiang¹; Janusz B Pawliszyn¹; ¹University of Waterloo, Waterloo, ON
- TP 156 **High-throughput end-to-end automated Evosep-MRM workflow for the quantification of glycated albumin in diabetes;** Bharath Kumar Raghuraman^{1,2}; Angela Mc Arde¹; Ole Vorm¹; Nicolai Bache¹; Martin Overgaard²; Christian Ravnsborg¹; ¹Evosep Biosystems, Odense, Denmark; ²Odense University Hospital, Odense, Denmark
- TP 157 **A fast and novel workflow with DART-LC-MSMS platform for urine toxicology screening and confirmation with orthogonal methods;** Francois Espourteille¹; Terry Bates²; ¹Bruker Corporation, Billerica, MA; ²Bruker Scientific, Billerica, MA
- TP 158 **FragFinder: Automatic selection of unique and selective EI fragment ions for GC-MS based metabolic screening;** Guan-yuan Chen^{1,2}; Ju-Yu Chen^{2,3}; Mei-Ling Lai²; Kun-Chen Lee^{2,4}; Te-I Weng^{1,2,5}; ¹Department and Graduate Institute of Forensic Medicine, College of Medicine, National Taiwan University, Taipei, Taiwan; ²Forensic and Clinical Toxicology Center, National Taiwan University Hospital, Taipei, Taiwan; ³Department of Pharmacy, College of Medicine, National Taiwan University, Taipei, Taiwan; ⁴Department of Laboratory Medicine, National Taiwan University Hospital, Taipei, Taiwan; ⁵Department of Emergency Medicine, National Taiwan University Hospital, Taipei, Taiwan
- TP 159 **Personalized extracellular vesicle phosphoproteomics identifies relevant functional signaling for renal cell carcinoma monitor;** Marco Hadisurya¹; Zhuojun Luo¹; Xiaofeng Wu²; Anton B. Iliuk³; Ronald S Boris⁴; W. Andy Tao^{1,3,5}; ¹Department of Biochemistry, Purdue University, West Lafayette, Indiana; ²Department of Chemistry, Purdue University, West Lafayette, Indiana; ³Tymora Analytical Operations, West Lafayette, Indiana; ⁴Department of Urology, Indiana University School of Medicine, Indianapolis, Indiana; ⁵Department of Chemistry, Purdue University, West Lafayette, Indiana
- TP 160 **Quantitation of endogenous steroids in serum using dried blood spot serum separator card and triple quadruple mass spectrometry;** Vikki Johnson¹; Nicholas Chestara²; Yoshiyuki Okamura³; ¹Shimadzu Scientific Instruments, Carlsbad, CA; ²DPX Technologies, La Jolla, CA; ³Shimadzu Scientific Instrument, Columbia, Maryland
- TP 161 **Rapid diagnosis of brain tumors by onco-metabolic detection using miniature mass spectrometry system;** Junhan Wu¹; Xinqi Fang²; Haoyue Zhang¹; Bin Jiao¹; Nan Wang³; Jiexun Bu³; Xiao Chen¹; Wei Hua²; Ying Mao²; Wenpeng Zhang¹; Zheng Ouyang¹; ¹Tsinghua University, Beijing, China; ²Huashan Hospital, Fudan University, Shanghai, China; ³PURSPEC Technology (Beijing) Ltd., Beijing, China
- TP 162 **Human Biofluid Benchmark Study comparing different workflows for deep and unbiased Clinical Proteomics;**

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- Carleen M Kluger¹; Giada Marino¹; Nagarjuna Nagaraj¹; Samira Vautrin¹; Till Kindel¹; Elena Kunold¹; Stefanie Tebbe¹; Frank Rolfs¹; Doris Staudt¹; Olga Shatnyeva²; Andreas Tebbe¹; ¹Evotec München GmbH, Neuried, Germany; ²Evotec International GmbH, Göttingen, Germany
- TP 163 **Kinetic study of trisulfide to disulfide conversion in IgG1 mAbs under physiological conditions using casirivimab and imdevimab as model molecules;** Lucy W Gao¹; Xuefei Zhong¹; Yuan Mao¹; Ning Li¹; Albert Torri²; ¹Analytical Chemistry Group, Regeneron Pharmaceuticals Inc., Tarrytown, New York; ²Bioanalytical Sciences, Regeneron Pharmaceuticals Inc., Tarrytown, New York
- TP 164 **Following molecular changes during wound skin healing with topical statin treatment;** Lilian Valadares Tose¹; Ahmed Hawash²; Ivan Jozic²; Francisco Fernandez-Lima¹; ¹Florida International University, Miami, FL; ²University of Miami, Miami, FL
- TP 165 **CardioCarePack – personalized medicine system to improve live quality of patients suffering from cardiac arrhythmias;** Maciej Stopa¹; Rafał Szewczyk^{1,2}; Anna Lenartowicz²; Julia Mironenka²; Katarzyna Krupczyńska - Krupczyńska - Stopa^{1,2}; Adrian Sobon^{1,2}; Leszek Kalinowski³; Adrianna Radulska³; Tomasz Borkowski³; Ewelina Marciniak³; ¹Bioanalytic Sp. z o.o., Gdansk, Poland; ²LabExperts sp. z o.o., Gdańsk, Poland; ³Gdansk Medical University, Gdansk, Poland
- TP 166 **Development and validation of a comprehensive liquid chromatography-tandem mass spectrometry-based test for plasma amino acid analysis in pediatric patients;** Lily Olayinka^{1,2}; Anil K Chokkalla^{1,2}; Deepthi Rajapakshe²; Emily Garnett^{1,2}; Sridevi Devaraj^{1,2}; ¹Department of Pathology and Immunology, Baylor College of Medicine, One Baylor Plaza, Houston, TEXAS; ²Department of Pathology, Texas Children's Hospital, Houston, Texas
- TP 167 **Higher Order Structure Characterization of a Monoclonal Antibody by Fast Photochemical Oxidation of Protein (FPOP)-Mass Spectrometry;** Yanchun Lin¹; Austin B. Moyle^{1,2}; Victor A. Beaumont³; Lucy L. Liu⁴; Sharon Polleck⁴; Don L. Rempel¹; Haijun Liu¹; Heliang Shi⁵; Jason C. Rouse⁴; Hai-Young Kim⁴; Ying Zhang^{4,6}; Michael L. Gross¹; ¹Washington university in St louis, St Louis, MO; ²AbbVie Inc., North Chicago, IL; ³Pfizer, Inc., Sandwich, United Kingdom; ⁴Pfizer, Inc., Andover, MA; ⁵Pfizer, Inc., New York City, NY; ⁶Sarepta Therapeutics, Inc., Cambridge, MA
- TP 168 **Mono- and Intralink Filter (Mi-Filter) To Reduce False Identifications in Cross-Linking Mass Spectrometry Data;** Xingyu Chen¹; Carolin Sailor¹; Kai Michael Kammer¹; Julius Fürsch¹; Eri Sakata²; Markus rainer Eisele²; Riccardo Pellarin³; Florian Stengel¹; ¹University of Konstanz, Konstanz, Germany; ²University Medical Center Göttingen, Göttingen, Germany; ³Institut Pasteur, Paris, France
- TP 169 **Chemoproteomic approaches to decipher novel mechanisms of non-vesicular cholesterol transport;** Miranda Villanueva¹; Nikolas Burton²; Andrew Palmer²; Sho Takechi²; Rohith Nagari²; Liujuan Cui²; Peter Tontonoz²; Keriann Backus²; ¹UCLA, LOS ANGELES, CA; ²UCLA, Los Angeles, CA
- TP 170 **Investigating daptomycin-membrane interactions using mass spectrometry;** Tapasyatanu Dash¹; Deseree Reid¹; Michael T Marty¹; ¹The University of Arizona, Tucson, Arizona
- TP 171 **New regions of interaction revealed for Aquaporin-0 binding partners via XL-MS;** Carla O'Neale¹; Zhen Wang¹; Kevin Schey¹; ¹Vanderbilt University, Nashville, TN
- TP 172 **A photo-tagging approach for studying the interactions between model peptides and membrane lipids;** Jing Zhao¹; Lipeng Qiao¹; Yu Xia¹; ¹Tsinghua University, Beijing, China
- TP 173 **In vitro to In vivo Characterization of Amyloid Beta 1-42 using Mass Spectrometry-based Footprinting;** Cynthia (xinyi) Kuang¹; Yanchun Lin¹; Zhao Sun²; Andrew Yoo²; Michael L. Gross³; ¹Washington University in St. Louis, St. Louis, MO; ²Washington University School of Medicine, St. Louis, MO; ³Washington university in St louis, St Louis, MO
- TP 174 **A New Tool in the Trans-Proteomic Pipeline for XL-MS Using Cleavable Cross-Linking Reagents;** Michael R. Hoopmann¹; David D. Shteynberg¹; Luis Mendoza²; Kamal Mandal²; Arun P. Wiita²; Eric W. Deutsch¹; Robert L. Moritz¹; ¹Institute for Systems Biology, Seattle, WA; ²University of California San Francisco, San Francisco, CA
- TP 175 **A Covalent Labeling-Mass Spectrometry Method for Identifying Protein Amyloid Inhibitors;** Kanitin Khamnong¹; Richard W. Vachet¹; ¹University of Massachusetts Amherst, Amherst, MA
- TP 176 **Optimized XL-MS workflows for membrane protein analysis;** Yi He¹; Gregory J Dodge²; Barbara Imperiali²; Rosa Viner¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Massachusetts Institute of Technology, Cambridge, MA
- TP 177 **Carbene Crosslinking in Gas-Phase Peptide Ion Scaffolds;** Hongyi Zhu¹; Václav Zima¹; Emily Ding¹; František Tureček¹; ¹University of Washington, Seattle, WA
- TP 178 **Dimethylthiourea as a Quencher in Hydroxyl Radical Protein Footprinting Experiments;** Anter A Shami¹; Sandeep K. Misra¹; Lisa Jones²; Joshua S. Sharp¹; ¹The University of Mississippi, University, MS; ²University of California San Diego, San Diego, CA
- TP 179 **A simple method for 'click-enabled' covalent labeling of hydrophobic protein microenvironments using radical mediated azidylation of amino acid sidechains;** Benjamin B. Minkoff¹; Heather L. Burch¹; Jamison D. Wolfer¹; Michael R. Sussman¹; ¹University of Wisconsin, Madison, WI
- TP 180 **Developing peptide-centric cleavable proximity labeling proteomics to study mitochondrial membrane protein topology;** Haorong Li¹; Jiawei Ni¹; Ryan Houston²; Shiori Sekine²; Ling Hao¹; ¹George Washington University, Washington, DC, DC; ²University of Pittsburgh, Pittsburgh, PA
- TP 181 **Conventional cell fixation improves performance of in situ crosslinking mass spectrometry while preserving ultrastructure;** Andrew RM Michael¹; Bruno C Amaral¹; David C Schriemer¹; ¹University of Calgary, Calgary, AB
- TP 182 **Confidently Identifying protein-protein interactions by harmonizing cross-link scores with machine learning;** Pin-Lian Jiang¹; Max Ruwolt¹; Boris Bogdanow¹; Fan Liu¹; ¹Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany
- TP 183 **Real-time library search improves the sensitivity and throughput of cross-link identification;** Max Ruwolt¹; Yi He²; Diogo Borges¹; William Barshop²; Rosa Viner²; Fan Liu¹; ¹Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; ²Thermo Fisher Scientific, San Jose, CA
- TP 184 **High-throughput XL-MS analysis on a new high-resolution accurate mass platform;** Yi He¹; Tabiwang Arrey²; Martin Zeller²; Nicolaie Eugen Damoc²; Rosa Viner¹; ¹ThermoFisher Scientific, San Jose, CA; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- TP 185 **Protein Footprinting Using Water Photolysis;** Oluwatosin A. Ogundairo¹; Kermit K. Murray¹; ¹Louisiana State University, Baton Rouge, LA
- TP 186 **Development of Fast Photochemical Footprinting of Glycans for Topographical Analysis of Glycans;** Sandeep K. Misra¹; Hao Liu¹; Sidney Stuckett¹; Joshua S. Sharp¹; ¹University of Mississippi, University, MS
- TP 187 **Cross-link assisted spatial proteomics to map sub-organelle proteomes and membrane protein topology;** Ying Zhu¹; Kerem Can Akkaya^{1,2}; Diogo Borges Lima¹; Max Ruwolt¹; Cong Wang¹; Martin Lehmann²; Fan Liu^{1,3}; ¹Department of Structural Biology, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP),

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- Berlin, Germany; ²Core Facility Cellular Imaging, Leibniz Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; ³Charité – Universitätsmedizin Berlin, Berlin, Germany
- TP 188 **Fluidic platform for enrichment of protein complexes for crosslinking-MS on a magnetic particle-based trap;** Shaunak Raval¹; David C Schriemer¹; Vladimir Sarpe¹; Alex D Crowder¹; Pauline Douglas¹; Susan P Lees-Miller¹; Danny Laurent¹; ¹University of Calgary, Calgary, AB
- TP 189 **Utilizing Diethylpyrocarbonate - Based Covalent Labeling Mass Spectrometry to Study Tau and Low-Density Lipoprotein Receptor-Related Protein 1 Binding and Interactions;** Vanessa L. Stahl¹; Zachary J. Kirsch²; Trisha W. Brady²; Andrew J. Shultz¹; Jennifer N. Rauch^{1,3}; Richard W. Vachet^{1,2}; ¹Molecular & Cellular Biology Program, University of Massachusetts Amherst, Amherst, MA; ²Department of Chemistry, University of Massachusetts Amherst, Amherst, MA; ³Department of Biochemistry & Molecular Biology, University of Massachusetts Amherst, Amherst, MA
- TP 190 **Are these crosslinking results significant? Bring on the bootstrap!**; Lindsey D Ulmer¹; Christopher N Woods²; Natalie L Stone²; Rachel E Klevit²; Matthew F Bush¹; ¹Department of Chemistry, University of Washington, Seattle, WA; ²Department of Biochemistry, University of Washington, Seattle, WA
- TP 191 **Thrombin-DNA Aptamer Binding Investigated by DEPC Covalent Labeling-MS;** Zachary J Kirsch¹; Jonathan Ashby²; Richard W. Vachet¹; ¹University of Massachusetts Amherst, Amherst, MA; ²Mount Holyoke College, Holyoke, MA
- TP 192 **Unique Protein Identifications Improve Protein-Protein Interaction Identification Rate in CRIMP 2.0;** D Alex Crowder¹; Vladimir Sarpe¹; David C Schriemer¹; ¹University of Calgary, Calgary, AB
- TP 193 **Few seconds range time-points for semi-automated Fenton Chemistry HRF reaction. Robust and inexpensive HOS monitoring method in vaccine antigen design;** Alessandro Vadi¹; Alessio Corrado¹; ¹GSK vaccines, Siena, Italy
- TP 194 **Accelerating Drug Discovery using an Automated High-Throughput Desorption Electrospray Ionization Mass Spectrometry Platform;** Nicolas M. Morato¹; Kai-Hung Huang¹; Samadhi C. Kulathunga¹; Veronica Feng¹; Beinan Yang¹; Jiang Yang¹; Eric T. Dziekonski¹; Timothy L. Ratliff¹; Andrew D. Mesecar¹; R. Graham Cooks¹; ¹Purdue University, WEST LAFAYETTE, IN
- TP 195 **Bioanalytical challenges and strategies to develop ultra-sensitive LC-MS/MS bioanalytical methods to quantify inhalation drugs in human plasma;** Min Meng¹; Laixin Wang¹; Yuhuan Ji¹; Zhong Hong¹; Aihua Liu²; ¹Chongqing Denali Medpharma, Beibei District, China; ²Alliance Pharma, Malvern, PA
- TP 196 **Quantitative Workflow for xC/UV/MS Data using a Single Vendor-Neutral Interface;** Anne Marie Smith¹; Yury Zhukov¹; Sofya Chudova¹; Vitaly Lashin¹; ¹ACD/Labs, Toronto, ON
- TP 197 **Development and validation of an LC-MS/MS method for quantitation of IACS-10759, a novel OxPhos inhibitor, in human plasma;** Quanyun Xu¹; Yongying Jiang¹; Emilia Di Francesco¹; Philip Jones¹; ¹Institute for Applied Cancer Science, UT MD Anderson Cancer Center, Houston, TX
- TP 198 **Developing Novel Bioanalytical Method for Direct Quantification of PEGylated Lipid CDN Nanodiscs in Mouse Serum Using LC-MS/MS and In-Source CID;** Ji Zhang¹; Eric L Dane²; Jianing Wang¹; ¹Millennium Pharmaceuticals, Inc., Cambridge, MA; ²Koch Institute for Integrative Cancer Research, Massachusetts Institute of Technology, Cambridge, MA
- TP 199 **Affinity Selection of Double-Click Triazole Libraries for Rapid Discovery of Allosteric Modulators for GLP-1 Receptor;** Ye Xin¹; Shuo Liu²; Karl Barry Sharpless³; Jiajia Dong²; Wenqing Shui¹; ¹ShanghaiTech University, Shanghai, China; ²Shanghai Jiao Tong University, Shanghai, China; ³The Scripps Research Institute, La Jolla, CA
- TP 200 **Intact mass analysis and kinetic models for ranking stabilizers of quaternary structure during drug development, and application to fALS;** Wensheng Yang¹; Md. Amin Hossain¹; Christopher Singleton¹; Brandon C. Miller¹; Yifan Liu¹; Roman Manestch¹; Jeffrey N. Agar¹; ¹Northeastern University, Boston, MA
- TP 201 **Towards Integrative Global, Phosphoproteomic and Metabolomic Profiling of Low-input Preparations of Spheroid-like Cells for Drug Discovery;** Norelle C. Wildburger¹; Cristina Di Poto¹; Jana Zecha¹; Mahder Abate^{1,2}; Silke Reisch³; Erik Allman¹; Lisa H. Cazares¹; Bilcan Bilada³; Sonja Hess¹; ¹AstraZeneca R&D, Gaithersburg, Maryland; ²University of Maryland College Park, College Park, MD; ³AstraZeneca, Molndal, Sweden
- TP 202 **Feasibility of nMS for large scale hit validation and screening through high compression;** Wenyi Hua¹; Xidong Feng¹; ¹Pfizer Inc., Groton, CT
- TP 203 **Mass Spectrometry-based Barcoding and Screening Platform Designed for Quantitative Macromolecular Drug Delivery;** Ning Wang¹; Nicole A. McNeer¹; Alex Kentsis^{1,2}; ¹Memorial Sloan Kettering Cancer Center, New York, New York; ²Weill Medical College of Cornell University, New York, New York
- TP 204 **Length distribution and content analysis of mRNA PolyA using MS and CE technique;** Xiaolei Lv¹; Tie Gao¹; Hexing Song¹; Luo Ji¹; Hongxu Chen¹; Lihai Guo¹; ¹SCIEX, China, Beijing, China
- TP 205 **Characterization of proteins in influenza virus vaccines by LC-MS/MS and CGE;** Xiaoxia Zhang¹; Yang Song¹; Ji Luo¹; Hongxu Chen²; ¹SCIEX, China, Shanghai, China; ²SCIEX, China, Beijing, China
- TP 206 **Deep proteomic screening and validation for systematic discovery of molecular glue compounds and novel degrader targets;** Uli Ohmayer¹; Martin Steger²; Bjoern Schwalb²; Anastasia Bednarz²; Sophie Machata²; Jutta Fritz²; Henrik Daub²; ¹NEOsphere Biotechnologies GmbH, Planegg, Germany; ²NEOsphere Biotechnologies GmbH, Planegg, Germany
- TP 207 **DRAFT: A Dose-Response Activity Finder Tool for drug target deconvolution in chemical proteomics experiments;** Praveen Kumar¹; Heng Zhao¹; Aarti Kawatkar¹; Steven Novick¹; ¹AstraZeneca, Waltham, MA
- TP 208 **Strategy for Bioanalysis of Liposomal Drugs in Support of Bioequivalence Study;** Yuhuan Ji¹; Jinzhi Liu¹; Min Meng¹; Xueyuan Zhang²; Chunlei Li²; Laixin Wang¹; ¹Chongqing Denali Medpharma Co.,Ltd, Chongqing, China; ²CSPC Pharmaceutical Group Ltd, Shijiazhuang, China
- TP 209 **RokaiXplorer: An online tool for interactive analysis of proteomics and phospho-proteomics data;** Serhan Yilmaz¹; Filipa Blasco Tavares Pereira Lopes¹; Marzieh Ayati²; Mark Chance¹; Mehmet Koyuturk¹; ¹Case Western Reserve University, Cleveland, OH; ²The University of Texas Rio Grande Valley, Edinburg, Texas
- TP 210 **Determination of BTK inhibitor concentration in patients with hematological diseases by HPLC-MS/MS;** Wenli Sun¹; Hongxing Liu¹; Jinyan Guo¹; Ran Xiao¹; Lei Wang¹; ¹Hebei Yanda Lu Daopei Hospital, Langfang, China
- TP 211 **Affinity selection mass spectrometry for high throughput drug screening of membrane proteins including GPCRs and solute carriers;** Kundan Sharma¹; Reda Assal¹; Shahid Rehan¹; Katharina Duerr¹; Laia Malet Sanz¹; Adam Sanderson¹; Jonathan Hopper¹; Steven Charlton¹; Ali Jazayeri¹; Ildir Liko¹; ¹OMass Therapeutics, Oxford, United Kingdom
- TP 212 **Unbiased validation of degrader drug neosubstrates by high-sensitivity slice-PASEF-mediated global ubiquitinomics;** Martin Steger¹; Uli Ohmayer¹; Bjoern

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- Schwalb¹; Jutta Fritz¹; Vadim Demichev²; Henrik Daub¹;
¹NEOsphere Biotechnologies GmbH, Planegg, Germany;
²Charité – Universitätsmedizin Berlin, Berlin, Germany
- TP 213 **LIP-MS combined with directDIA+ allows for highly specific drug target deconvolution**; Monika Pepelnjak¹; Fabio Sabino¹; Jaruschka Pecnik¹; Roland Bruderer¹; Tejas Gandhi¹; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland
- TP 214 **Development of a robust covalent fragment screening platform using data independent acquisition (DIA) mass spectrometry**; Gregory K. Potts¹; Alex Shannon¹; Ryan A. McClure¹; Adam Banlasan¹; Hua Tang¹; Violeta Marin¹; Janice Lee¹; Noah P. Tu¹; Jon D. Williams¹; Anil Vasudevan¹; ¹AbbVie, Inc., North Chicago, IL
- TP 215 **Coupling thermal shift assay sample preparation with 2D-LCMS as a tool for determining in vivo drug-protein target engagement**; Bao-Jen Shyong¹; Matthew T. Mazur²; Qian Huang²; Carl J. Balibar²; Weixun Wang²; ¹Merck & Co. Inc., West Point, PA; ²Merck & Co., Inc., West Point, PA
- TP 216 **Real-time batch LC-MS and NMR data processing and LIMS reporting for small molecule characterization**; Sarah Robinson¹; Kewei Xu¹; ¹Genentech, Inc, South San Francisco, CA
- TP 217 **DrugMap: A Pan-Cancer Analysis of Protein Druggability**; Siwen Zhang¹; Mariko Hara¹; Harrison Byron Chong¹; Liron Bar-Peled¹; ¹MGH, Boston, MA
- TP 218 **A High Throughput QC Method for Assessing Serial Dilution Performance of Dose-Response Plates**; Lei Yang¹; Mary Rimmer¹; Kendall Billingsley¹; Kaylee Bundy¹; Mariana Santana Ponce¹; Shalandus Garrett¹; Chepyala Divyabharathi¹; Yong Li¹; Mitchell Sharnise¹; Currier Duane¹; Bryan Julianne¹; Rankovic Zoran¹; ¹St. Jude Children's Research Hospital, Memphis, Tennessee
- TP 219 **Measuring Chromatography Column Effect on Mass Spec Feature Coelution and Deconvolvability**; Lizzie Spencer¹; Laurel D. Wright¹; Thomas Butler¹; John T. Prince¹; David Healey¹; ¹Enveda Biosciences, Boulder, CO
- TP 220 **Elucidation of Novel Per- and Polyfluoroalkyl Substances (PFAS) Using a Non-Targeted LC-IMS-MS Method with Size-Dependent Fragmentation**; Kaylie I Kirkwood¹; James N Dodds²; Erin S Baker²; ¹North Carolina State University, Raleigh, NC; ²University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 221 **Pushing PFAS Possibilities: The Hunt for Ultra Sensitivity to Reach ppq EPA Health Advisory Levels**; Ken Rosnack¹; Kari Organtini¹; Henry Foddy²; Nicola Dreolin²; Stuart Adams²; Peter Hancock²; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Wilmslow, United Kingdom
- TP 222 **Proteomic profiling and comprehensive analysis of the ecotoxicity mechanisms of zebrafish embryos in response to benzyl benzoate**; Young Sang Kwon¹; Seung-Min Lee¹; Yeong-Jin Kim¹; Yoon-Jeong Jeon¹; Wenting Wang¹; Jong-Su Seo¹; Jong-Hwan Kim¹; ¹Environmental Safety Assessment Center, Gyeongnam Branch Institute, Korea Institute of Toxicology, Jinju, South Korea
- TP 223 **Strategies for Ultimate Sensitivity of Per- and Polyfluoroalkyl Substances (PFAS) in Water**; Emily Parry¹; David A Weil²; Patrick Batoon²; Tarun Anumol¹; ¹Agilent Technologies, Wilmington; ²Agilent Technologies, Santa Clara, CA
- TP 224 **Real-time detection of health-relevant substances and pollution sources using novel technologies in single-particle mass spectrometry**; Johannes Passig¹; Julian Schade^{1,2}; Ellen Iva Rosewig¹; Lukas Alexander Anders¹; Robert Irsig³; Sven Ehler³; Andreas Walte³; Ralf Zimmermann¹; ¹Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; ²University of Bundeswehr Munich, Faculty for Mechanical Engineering, Institute of Chemical and Environmental Engineering, Neubiberg, Germany; ³Photonion GmbH, Schwerin, Germany
- TP 225 **High Resolution-MS uncovers new halocyclopentadiene disinfection by-products in drinking water**; Susan Richardson¹; Jiafu Li^{1,2}; Md. Tareq Aziz¹; Caroline Granger¹; ¹University of South Carolina, Columbia, SC; ²Soochow University, Suzhou, China
- TP 226 **Evaluating detectability as LoD from the predicted ionization efficiency values for ESI+ and ESI-**; Amina Souihri¹; Jonathan Martin²; Anneli Kruve¹; ¹Department of Environmental and Materials Chemistry, Stockholm University, Stockholm, Sweden; ²Department of Environmental Science, Stockholm University, Stockholm, Sweden
- TP 227 **LC-MS/MS combined with complimentary methods to quantify total PFAS concentration in contaminated water**; Leif Abrell¹; Osmar Luiz Moreira P F Menezes¹; Kartika Srivastava¹; Danielle Barrientes¹; Jon Chorover¹; Reyes Sierra Alvarez¹; ¹University of Arizona, Tucson, AZ
- TP 228 **Functional group analysis of gas-phase oxidation products of α -pinene using high resolution collision-induced dissociation mass spectrometry**; Daisuke Fukuyama¹; Kanako Sekimoto¹; ¹Yokohama City University, Yokohama-shi, Japan
- TP 229 **Mass Spectrometry tools for confident discrimination of different qualities of post-consumer recycled plastics**; Hania Khoury-Hollins¹; Bryan Katzenmeyer²; Rachel J Sanig³; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters corp, milford, MA; ³Waters Corporation, Wilmslow, United Kingdom
- TP 230 **An ultra-high sensitivity analysis approach for detecting PFAS compounds in water sources**; Jianru Stahl-Zeng¹; Bertram Nieland²; Jack Steed³; Abdessamad Chahbouni⁴; ¹SCIEX, Darmstadt, Germany; ²SCIEX, Darmstadt, Germany; ³SCIEX, Macclesfield, United Kingdom; ⁴Het Water Lab, J.W. Lucasweg 2 2031 BE Haarlem, Netherlands
- TP 231 **Comprehensive Analytical Workflow of PFAS Analysis in Aqueous Environmental Samples**; Ying Long¹; Ana Ramos¹; James Smalley¹; Lam Leung¹; ¹Chemours, NEWARK, DE
- TP 232 **Analysis of organic chemicals in aerosol particulate matter in Mongolia using high-throughput UPLC FT-ICR MS and artificial neural network**; Seungwoo Son¹; Moonhee Park²; Young Hwan Kim²; Sunghwan Kim^{1,3}; ¹Kyungpook National University, Daegu, South Korea; ²Korea Basic Science Institute, Cheongju, South Korea; ³Mass Spectrometry Converging Research Center and Green-Nano Materials Research Center, Daegu, South Korea
- TP 233 **Microplastic Analysis and Additive Screening using Thermal Desorption/Pyrolysis DART-MS**; William L Fatigante¹; Sam Putnam¹; Kushal Modi¹; ¹Bruker Scientific, LLC, Billerica, MA
- TP 234 **Analysis of PAHs Using the Hydrogen-Optimized Source with GC/MS and GC/MS/MS in Challenging Soil Matrix**; Samuel P Haddad¹; Bruce D Quimby¹; Anastasia A Andrianova¹; Eric L Fausett¹; ¹Agilent Technologies, Wilmington, DE
- TP 235 **Blow flies as remote sampling devices: Detection of insensitive munitions and their degradation products in the environment using LC-MS/MS**; Sarah Dowling¹; Sarah Prunty¹; Katie Jensen¹; Christine Picard¹; Nicholas Manicke¹; ¹Indiana University Purdue University Indianapolis, Indianapolis, IN
- TP 236 **Reduction of PFAS in Drinking Water using a Filter containing Activated Carbon plus Ion Exchange Resin, measured using QSight LC-MS/MS**; Cole Stratman¹; Jacob Jalali²; Jesse Leonard²; Erasmus Cudjoe³; Marc R Elie²; ¹PerkinElmer, Charlestown, RI; ²PerkinElmer, Shelton, CT; ³PerkinElmer Inc., Woodbridge, ON

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- TP 237 **Evaluating Known and Novel PFAS in Firefighter Blood with Non-Targeted Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry Measurements;** Ashlee T Falls¹; Anna Boatman¹; Kaylie Kirkwood²; Heather M Stapleton³; Erin S Baker¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC; ²North Carolina State University, Raleigh, NC; ³Duke University, Durham, NC
- TP 238 **Unravelling the biological impacts of PFAS contamination using omics-based mass spectrometry ecosurveillance techniques in wild-caught freshwater turtles;** David J. Beale¹; Thomas Nguyen¹; Utpal Bose²; Jordi Nelis²; Sally Stockwell²; James A. Broadbent²; Matthew C. Smith³; Andrew Bissett³; Gunjan Pandey⁴; Leon Court⁴; Rahul Rane⁵; Caitriona Walsh⁴; Nicholas Bourne²; Sandra Nilsson⁶; Viviana Gonzalez-Astudillo⁷; Christoph Braun⁸; Brenda Baddiley⁸; Stephanie Shaw⁸; Josh Llinas⁹; Duncan Limpus⁸; Suzanne Vardy⁸; ¹CSIRO, Dutton Park, Australia; ²CSIRO, St Lucia, Australia; ³CSIRO, Hobart, Australia; ⁴CSIRO, Canberra, Australia; ⁵CSIRO, Parkville, Australia; ⁶The University of Queensland, Woollongabba, Australia; ⁷The University of Queensland, Gatton, Australia; ⁸Queensland Department of Environment and Science, Dutton Park, Australia; ⁹Unusual Pets Veterinarian, Brisbane, Australia
- TP 239 **PY-GCMS analysis of microplastics in environmental samples using nitrogen as an alternative carrier gas;** Andy Sandy¹; Evelyn Wang²; Ruth Marfil-Vega²; Yoshiyuki Okamura²; ¹Shimadzu Scientific Instruments, Columbia, MD; ²Shimadzu Scientific Instrument, Columbia, Maryland
- TP 240 **Identification of a Serine-containing Microcystin by Thiol Derivatization and Specific MS/MS Neutral Losses;** Sanduni H Premathilaka¹; Johnna A Birbeck²; Judy A Westrick²; Dragan Isailovic¹; ¹University of Toledo, Toledo, OH; ²Wayne State University, Detroit, MI
- TP 241 **Characterizing the Isomeric Forms of PFASs in Biological Samples with UHPLC and Ion Mobility Mass Spectrometry;** Carrie A McDonough¹; David Dukes²; Jennifer Marciano²; Emily Parry³; David A Weil³; Sheher Banu Mohsin³; ¹Carnegie Mellon University, Pittsburgh, PA; ²Stony Brook University, Stony Brook, NY; ³Agilent Technologies, Santa Clara, CA
- TP 242 **Accurate mass library for PFAS analysis in environmental samples using high resolution GC/Q-TOF;** Sofia Nieto¹; Matthew Giardina¹; Luann Wong²; Gabrielle Black²; Thomas Young²; ¹Agilent Technologies, Inc., Santa Clara, CA; ²Department of Civil and Environmental Engineering, UC Davis, Davis, CA
- TP 243 **Suspect Screening of Organic Contaminants in Nutraceuticals with Ultra-high Performance Liquid Chromatography/Quadrupole Time-of-flight Mass Spectrometry;** Hung-Ju Shih¹; Chia-Yang Chen¹; ¹Institute of Food Safety and Health, College of Public Health, National Taiwan University, Taipei City, Taiwan
- TP 244 **Integrated and Quantitative Multi-omic Method for analyzing the macronutrients of Food using Rapid-Throughput LC-MS;** Chongye (shawn) Ehlers Cheang¹; Cheng-Yu Weng¹; Garret Couture¹; Carlito B. Lebrilla¹; ¹University of California, Davis, Davis, CA
- TP 245 **Quantitative Analysis of Anthocyanins in Plant Materials by LC-DAD-MS with Molar Relative Response Factors (MRRFs);** Wen Dong¹; Xin Yang¹; Ning Zhang²; Pei Chen³; Jianghao Sun³; James Harnly³; Mengliang Zhang⁴; ¹Middle Tennessee State University, Murfreesboro, TN; ²Fisk University, Nashville, TN; ³USDA-ARS, Beltsville, MD; ⁴MTSU, Murfreesboro, TN
- TP 246 **Intact mass characterization reveals novel post-translationally cleaved allergenic proteins from peanut;** Justin Marsh¹; Danijela Apostolovic²; Govardus De Jong³; Stef J Koppelman¹; Philip Johnson¹; ¹University of Nebraska Lincoln, Lincoln, NE; ²Karolinska Institute, Solna, Sweden; ³Wageningen University, Wageningen, Netherlands
- TP 247 **LC-MS/MS method for quantifying glycerol monolaurate (GML) isomers in human milk: development, validation, and relevant pilot study findings;** Thomas Vennard¹; Nathan A. Meredith¹; Michael Gray¹; Sarah Maria¹; Shay Phillips¹; Lauren Brink²; Ruth Simmons³; ¹Mead Johnson Nutrition, Evansville, IN; ²Reckitt, Parsippany, NJ; ³Reckitt, Slough, United Kingdom
- TP 248 **Quality Discrimination of Jasmine Tea using LC-Q/TOF Combined with Sensory Evaluation and Statistical Method;** Xinwei Feng¹; Jason Li¹; Nola Yu¹; ¹APTC, The Coca-Cola Company, Shanghai, China
- TP 249 **HPLC-MS based chemical profiling of bioactive compounds in Black Garlic and its extracts;** Alberto AA Asteggiano^{1,2}; Alessandra Porcu³; Andrea Occhipinti³; Valentina Schiavo¹; Claudio Medana¹; ¹University of Turin, Dipartimento di Biotecnologie Molecolari e Scienze per la Salute, Turin, Italy; ²Biosfered S.R.L., Turin, Italy; ³Abel Nutraceuticals, Turin, Italy
- TP 250 **Proteomics of Western Honeybees to Assess Colony Health;** Vincent Riciglionio¹; Taylor Bell²; Ally Martin¹; Fabrizio Donnarumma²; Kermit K. Murray²; ¹USDA-ARS, Honey Bee Breeding, Genetics, and Physiology Research, Baton Rouge, Louisiana; ²Louisiana State University, Baton Rouge, LA
- TP 251 **Optimization of extraction method to determine 12 novel brominated flame retardants in squid using gas chromatography-tandem mass spectrometry;** Eunbin Bae¹; Sun Kyoung Joung¹; Hamin Choi¹; Sang Beom Han¹; ¹Chung-Ang University, Seoul, South Korea
- TP 252 **High-resolution mass spectrometry (HRMS) method for determine 43 per- and polyfluoroalkyl substances (PFAS) in vegetables;** Gui-Ru Xie¹; HONG-JHANG Chen¹; ¹Institute of Food Science and Technology, National Taiwan University, Taipei, Taiwan
- TP 253 **Determination of chemically induced deamidation sites of gluten peptides using ion mobility or ultra-high resolution mass spectrometry;** Matthew E Daly¹; Qianying Xu²; Si Cheng³; Lisa Reid¹; Lee A Gettings¹; Emma Marsden-Edwards¹; E NC Mills^{2,4}; ¹Waters Corporation, Wilmslow, United Kingdom; ²University of Manchester, Manchester, United Kingdom; ³Waters Corporation, Costa Mesa, CA; ⁴University of Surrey, Guildford, United Kingdom
- TP 254 **Application Of Liquid Chromatography–Mass Spectrometry And Species And Tissue Specific Peptide Biomarkers To Food Authentication And Detection Of Adulterations;** Emilia Fornal¹; Anna Stachniuk¹; Magdalena Montowska²; Agata Sumara¹; Alicja Trzpił¹; ¹Medical University of Lublin, Lublin, Poland; ²Poznan University of Life Sciences, Poznan, Poland
- TP 255 **Quantitative Determination of Cannabidiol (CBD) Derivatives in Hemp Containing Products by Nano LC-MS/MS;** Md Mostofa Al Amin Bhuiyan¹; Cristian D. Gutierrez Reyes¹; Waziha Purba¹; Andrew Bennett¹; Sherifdeen Onigbinde¹; Adeniyi Moyinoluwa¹; Yehia Mehref¹; ¹Texas Tech University, Lubbock, Texas
- TP 256 **Development of LC-MS method for quantification of Aflatoxin M1 in human urine samples;** Gabriela Ávila-Villarreal^{1,2}; Candy Andreina Montaña-Pérez¹; Guadalupe Yáñez-Ibarra¹; Jorge-Luis Figueroa-Cordova^{1,3}; Cyndia-Azucena González-Arias³; ¹Unidad Especializada en I+D+i Calidad de Alimentos y Productos Naturales, Centro Nayarita de Innovación y Transferencia de Tecnología A.C., Tepic, Mexico; ²Unidad Académica de Ciencias Químico Biológicas y Farmacéuticas, Universidad Autónoma de Nayarit, Tepic, Mexico; ³Laboratorio de Contaminación y Toxicología Ambiental, Universidad Autónoma de Nayarit, Tepic, Mexico
- TP 257 **Characterization of Unsaturated Fatty Acids in Negative OAD-MS/MS using LCMS-9050;** Hidenori Takahashi¹; Mami Okamoto¹; Yuta Miyazaki¹; Yohei Arai¹; Natsuyo Asano¹; ¹Shimadzu Corporation, Kyoto, Japan

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- TP 258 **Applications of LC-MS to analyze food-derived bioactive peptides: from food processing to simulated gastrointestinal digestion;** Yu-Ping Huang¹; Fernanda Furlan Goncalves Dias¹; Juliana Maria Leite Nobrega De Moura Bell¹; Daniela Barile¹; ¹University of California Davis, Davis, CA
- TP 259 **Rapid-throughput Automated Sample Preparation for Human Milk Oligosaccharides Analysis Using an Open-source Liquid Handler;** Aaron D Stacy¹; Anita Vinjamuri¹; Carlito B. Lebrilla¹; ¹UC Davis, Davis, CA
- TP 260 **Onions, Garlic and FODMAPs: Characterization of Fructan Structure and Hydrolytic Effects of Microbial Inulinase Using LC-MS;** James G Farmer¹; Justin L Guice¹; Morgan D Hollins¹; Kelly T Tinker¹; Sean M Garvey¹; ¹BIO-CAT, Troy, VA
- TP 261 **Analysis of fatty acid content in rice by GC-MS/MS combined with metabolite database;** Yong Wang¹; Jun Fan²; ¹Shimadzu Enterprise Management (China) Co., Ltd, Beijing, China; ²Shimadzu Enterprise Management (China) Co., Ltd, Shanghai, China
- TP 262 **Non-targeted liquid phase high resolution mass spectrometry detection method for soy sauce additives;** Ye Geng; Shaanxi University of Science and Technology, Xi'an, China
- TP 263 **Development of an arsenic speciation method to explore phytomanagement potential of hemp;** Rachel R Jones¹; Jacqueline Michelle Chaparro¹; Tyler J Richards¹; Jessica Prenni¹; ¹Colorado State University, Fort Collins, CO
- TP 264 **Protein Structure Elucidation from Mass Spectrometry Data using Rosetta and AlphaFold;** Steffen Lindert; The Ohio State University, Columbus, OH
- TP 265 **Binding of Inhibitors on Aβ42: Application of DFT Calculations and Fast Photochemical Oxidation Mass Spectrometry;** George Mathai¹; Cynthia (xinyi) Kuang²; Saketh Chemuru³; Daryl Giblin²; Michael L. Gross³; ¹Emeritus - Sacred Heart College, Kochi, India; ²Washington University in St. Louis, St. Louis, MO; ³Washington university in St Louis, St Louis, MO
- TP 266 **MALDI coupled with negative ion electron capture dissociation (niECD) for characterization of labile acidic biomolecules;** Steven A. Defiglia¹; Kristina Hakansson¹; ¹University of Michigan Ann-Arbor, Ann Arbor, MI
- TP 267 **Free OH Radicals Selectively Oxidize Heterocycles under APCI-MS;** Dmitry Eremin¹; Shubhangi Aggarwal¹; Valery Fokin¹; ¹University of Southern California, Los Angeles, CA
- TP 268 **Investigating the gas-phase structural dynamics of amyloid-β and its complex with a chelating neuropeptide in the presence of copper ions;** Despoina Svingou¹; Ri Wu¹; Lukas Raphael Benzenberg¹; Renato Zenobi¹; ¹ETH Zurich, Zurich, Switzerland
- TP 269 **Stabilization of fragment ions on surfaces: understanding the reactivity of undercoordinated metal complexes in the condensed phase using ion soft-landing;** Hugo Y Samayoa-Oviedo¹; Robert Schiewe²; Harald Knorke²; Jonas Warneke^{2,3}; Julia Laskin¹; ¹Purdue University, West Lafayette, Indiana; ²Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, Leipzig University, Leipzig, Germany; ³Leibniz Institute of Surface Engineering (IOM), Leipzig, Germany
- TP 270 **Use of Visualized Rayleigh Limit to Aid in Charge Detector Calibration;** David Hrabovsky¹; Richard B. Cole²; ¹Sorbonne Université, Faculté des Sciences et de l'Ingénierie, Paris, France; ²Sorbonne Université, Faculté des Sciences et de l'Ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France
- TP 271 **Activation and Relaxation of Protein Ions Observed Using Time-Resolved Ion-Neutral Collision Cross Sections in an FT-ICR MS;** Savannah R Porter¹; Noah J Mismash¹; Andrew J Arslanian^{1,2}; David V Dearden¹; ¹Brigham Young University, Provo, UT; ²The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH
- TP 272 **Factors Controlling Ion Yields in Droplet Assisted Ionization;** Jim Walker¹; Kelvin Risby¹; Oli Boswell¹; Amaran Varma¹; Joshua Harrison¹; Bryan R Bzdek¹; ¹University of Bristol, Bristol, United Kingdom
- TP 273 **Bismuth-Mediated Capture of the Cysteine-Rich Dark Proteome in Mycobacteria;** Hannah A. Marietta¹; C. Bruce Mousseau¹; Matthew M. Champion¹; ¹University of Notre Dame, Notre Dame, IN
- TP 274 **Structural studies on somatostatin and octreotide in the presence of copper ions by means of FRET and ion mobility spectrometry;** Lukas Raphael Benzenberg¹; Ri Wu¹; Despoina Svingou¹; Renato Zenobi¹; ¹ETH Zurich, Zurich, Switzerland
- TP 275 **Microdroplet Mass Spectrometry-based Method for Detecting Hemoglobin Adducts;** Hung-Hsiang Jen¹; Kang-Yu Liu¹; Shu-Hui Chen¹; Chin-Ming Kuo¹; Fung-Yu Chen¹; ¹National Cheng Kung University, Tainan, Taiwan
- TP 276 **Isotopocules of Oxanions: A Journey from Ice Cores to Humans;** Cajetan Neubauer¹; Kristýna Kantnerová¹; Sebastian Kopf¹; Andreas Hilkert²; ¹University of Colorado Boulder, Boulder, CO; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- TP 277 **Dissecting the formation of protein corona on nanoparticles allows reconstructing deep plasma protein concentrations and discovering novel proteoforms;** Alexey Stukalov¹; Shadi Ferdosi¹; Yingxiang Huang¹; Moaraj Hasan¹; Brittany Lee¹; Asim Siddiqui¹; Serafim Batzoglou¹; Daniel Hornburg¹; ¹Seer Inc., Redwood City, CA
- TP 278 **High-efficiency survey of analytes enabled by modulated ion transfer and MS/MS analysis;** Xiaomin Fan¹; Zheng Ouyang¹; ¹Department of Precision Instrument, Tsinghua University, Beijing, China
- TP 279 **Advances in molecular analysis at the nanoscale;** Thanh Loan Lai¹; Dmitriy S. Verkhoturov¹; Michael J. Eller²; Serge Della Negra³; Stanislav V. Verkhoturov¹; Emile A. Schweikert¹; ¹Department of Chemistry, Texas A&M University, College Station, TX; ²Department of Chemistry and Biochemistry, California State University Northridge, Northridge, CA; ³University of Paris-Saclay, CNRS/IN2P3, IJCLab, Orsay, France
- TP 280 **Mucinase S_mE enables improved glycoproteomic mapping of mucin-domain glycoproteins;** Alexandra Steigmeyer¹; Joann Chongsaritsinsuk¹; Keira E. Mahoney¹; Taryn M. Lucas¹; Deniz Ince¹; Alexandria Battison¹; Marie A. Hollenhorst²; D. Judy Shon²; Victor Attah¹; Catherine Kwon¹; Carolyn R. Bertozzi²; Stacy A. Malaker¹; ¹Yale University, New Haven, CT; ²Stanford University, Stanford, CA
- TP 281 **Exposing the molecular heterogeneity of glycosylated biotherapeutics;** Luis F Schachner¹; Christopher Mullen²; Wilson Phung¹; Joshua Hinkle²; Michelle Irwin Beardesley¹; Tracy Bentley¹; Peter Day¹; Christina Tsai¹; Siddharth Sukumaran¹; Tomasz Baginski¹; Danielle Dicara¹; Nicholas Agard¹; Matthieu Masureel¹; Joshua Gober¹; Adel Elsohly¹; John E.P. Syka²; Romain Huguet²; Michael T Marty³; Wendy Sandoval¹; ¹Genentech Inc, South San Francisco, CA; ²Thermo Fisher Scientific, San Jose, California; ³University of Arizona, Tucson, AZ
- TP 282 **Glycan-dependent Affinity Purification Mass Spectrometry (GAP-MS) provides novel insights into glycoprotein interaction network;** Yixuan (axe) Xie¹; Xingyu Liu¹; Siyu Chen²; Zongtao Lin¹; Carlito B. Lebrilla²; Benjamin A Garcia¹; ¹Washington University School of Medicine, St. Louis, MO; ²University of California, Davis, Davis, CA
- TP 283 **All in One: Direct Site-specific Detailed Glycan Characterization by Higher Energy Electron Activated Dissociation Tandem Mass Spectrometry;** Ruiqing Li¹; Chaoshuang Xia²; Haowei Tong¹; Weiwei Wang¹; Catherine

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- E. Costello²; Cheng Lin²; Juan Wei¹; ¹Shanghai Jiao Tong University, Shanghai, China; ²Boston University Chobanian and Avedisian School of Medicine, Boston, MA
- TP 284 **Large-scale and Site-specific Mapping of the Murine Brain O-Glycoproteome with IMPa; Suttipong Suttapitugsakul¹; Yasuyuki Matsumoto¹; Rajindra P Aryal¹; Richard D Cummings¹; ¹Department of Surgery, Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, MA**
- TP 285 **Correlating glycoform and structural heterogeneity of the intact SARS-CoV-2 receptor binding domain with ultraviolet photodissociation and collision cross section analysis; Virginia K James¹; Katelynn S. Zuercher¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX**
- TP 286 **Optimization of Methods for Building Human Glycopeptide Libraries; Yi Liu¹; Meghan C. Burke¹; Zachary C. Goecker¹; Sergey L. Sheetlin¹; Guanghui Wang¹; Yuxue Liang¹; Zheng Zhang¹; Yuri A. Mirokhin¹; Xiaoyu Yang¹; Dmitrii V. Tchekhovskoi¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD**
- TP 287 **N-Glycosylation Profile of EpCAM in Epithelial and Breast Cancer Cells; Nicole M. Jenkinson¹; Lauren R. DeVine^{2,3}; Caitlin M. Tressler¹; Robert N. Cole^{2,3}; Kristine Glunde^{1,3,4}; ¹Russell H. Morgan Department of Radiology and Radiological Science, Division of Cancer Imaging Research, Johns Hopkins University School of Medicine, Baltimore, MD; ²Mass Spectrometry and Proteomics Facility, Johns Hopkins University School of Medicine, Baltimore, MD; ³Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD; ⁴Sidney Kimmel Comprehensive Cancer Center, Johns Hopkins University School of Medicine, Baltimore, MD**
- TP 288 **Variation of Site-Specific Glycosylation Profiles for Influenza Glycoproteins from Different Vaccines and Recombinant Sources; Zachary C Goecker¹; Meghan C. Burke¹; Concepcion A. Remoroza¹; Yi Liu¹; Yuri A. Mirokhin¹; Sergey L. Sheetlin²; Dmitrii V. Tchekhovskoi¹; Xiaoyu Yang¹; Stephen E. Stein¹; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²National Institute for Standards and Technology, Gaithersburg, MD**
- TP 289 **In-depth O-glycosylation characterization and comparison of commercially available etanercept products using the ZenoTOF 7600 system; Wang Wentao¹; Song Hexing²; Luo Ji³; Chen Hongxu²; Guo Lihai⁴; ¹Sciex, Guangzhou, China; ²SCIEX, Beijing, China; ³SCIEX, Shanghai, China; ⁴SCIEX, Beijing, China**
- TP 290 **One-step preparation of boric acid-riched hydrothermal spheres for N-glycopeptides analysis in preeclampsia serum; Yinghua Yan¹; Chuan-Fan Ding¹; ¹Ningbo University, Ningbo, China**
- TP 291 **Characterizing Reproducibility of Glycoform Distributions for SARS-CoV-2 Spike Protein-Derived Glycopeptides Across Recombinant Protein Sources Using Automated, Mass Spectral Library-Based Methods; Meghan C. Burke¹; Yi Liu¹; Concepcion A. Remoroza¹; Yuri A. Mirokhin¹; Sergey Sheetlin¹; Dmitrii V. Tchekhovskoi¹; Guanghui Wang¹; Xiaoyu Yang¹; Stephen E. Stein¹; ¹National Institute of Standards and Technology, Gaithersburg, MD**
- TP 292 **Introducing the GlycoPaSER prototype for real-time N-glycopeptide identification on the PaSER platform; Gad Armony¹; Sven Brehmer²; Tharan Srikumar³; Lennard Pfenning²; Fokje Zijlstra⁴; Dennis Trede²; Gary Kruppa⁵; Dirk Lefeber^{4,6}; Alain Van Gool⁴; Hans Wessels⁴; ¹Translational Metabolic Laboratory, Department of Laboratory Medicine, Radboud Institute for Molecular Life Sciences, RadboudUMC, Nijmegen, Netherlands; ²Bruker Daltonics, Bremen, Germany; ³Bruker Ltd, Milton, ON; ⁴Translational Metabolic Laboratory, Department of Genetics, Radboud Institute for Molecular Life Sciences, RadboudUMC, Nijmegen, Netherlands; ⁵Bruker S.R.O., Brno, Czech Republic; ⁶Department of Neurology, Donders Institute for Brain, Cognition and Behavior, RadboudUMC, Nijmegen, Netherlands**
- TP 293 **Mass spectrometry characterization of N-glycosylation and disulfide bonds of the spike protein from SARS-CoV-2 Omicron variant; Dongxia Wang¹; Jakub Baudys¹; Sarah H. Osman²; John R Barr¹; ¹Centers of Disease Control and Prevention (CDC), Atlanta, GA; ²Centers for Disease Control and Prevention, Atlanta, GA**
- TP 294 **Characterization of the site specific N- and O-glycosylation of proteins using LC-MS/MS analysis and the I-GPA platform; Ju Yeon Lee^{1,2}; Jin-Woong Choi^{1,3}; Sanghyeon Bae¹; Heeyoun Hwang^{1,2}; Young Ho Jeon⁴; Jin Young Kim^{1,2}; ¹Korea Basic Science Institute, Cheongju, South Korea; ²Korea Research Institute of Bioscience and Biotechnology, Yuseong-gu, South Korea; ³Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; ⁴Korea university, Sejong, South Korea**
- TP 295 **High-resolution MS-based multiproteomic analysis of esophageal cancer lines reveal potential link between estrogen signaling and esophageal cancer; Chao Peng¹; Jingzhi Zhao¹; Ping Wu¹; Gunagqing Chen¹; Lukang Sun¹; Jing Huang¹; Jun Ma¹; Wenting Li¹; Baozhen Shan¹; ¹BaizhenBio Inc., shanghai, China**
- TP 296 **Fragment ion triggered Parallel Accumulation SERIAL Fragmentation stepping for enhanced glycoproteomics data acquisition and beyond; Gad Armony¹; Michael Krause²; Pierre-Olivier Schmit³; Dennis Trede²; Gary Kruppa⁴; Dirk Lefeber^{1,5}; Alain Van Gool¹; Hans Wessels¹; ¹Translational Metabolic Laboratory, Department of Laboratory Medicine, Radboud Institute for Molecular Life Sciences, RadboudUMC, Nijmegen, Netherlands; ²Bruker Daltonics GmbH & Co.KG, Bremen, Germany; ³Bruker Daltonique S.A., Wissembourg, France; ⁴Bruker S.R.O., Brno, Czech Republic; ⁵Department of Neurology, Donders Institute for Brain, Cognition and Behavior, RadboudUMC, Nijmegen, Netherlands**
- TP 297 **Regulation of Protein N-linked Glycosylation Site Occupancy.; Marium Khaleque¹; Amanda S. Nouwens¹; Benjamin L. Schulz¹; ¹The University of Queensland, Brisbane, Australia**
- TP 298 **Quantitative glycoproteome analysis using a novel nanoparticle-based plasma proteomics workflow; Shadi Ferdosi¹; Moaraj Hasan¹; Iman Mohtashemi¹; Evan O'Brien¹; Hongwei Wang¹; Jian Wang¹; Khatereh Motamedchaboki¹; Harendra Guturu¹; Daniel Hornburg¹; ¹Seer, Inc., Redwood City, CA**
- TP 299 **Correlating LC-MS/MS glycomic, glycoproteomic, and transcriptomic data to determine glycosylation pathways in lung cancer; Michael Russelle S Alvarez¹; Patrick Moreno²; Armin Oloumi¹; Ryan Lee Schindler¹; Qingwen Zhou¹; Michelle Narciso³; Sheryl Joyce B. Grijaldo³; Ruel C. Nacario³; Gladys C. Completo³; Francisco M. Heralde III²; Carlito B. Lebrilla¹; ¹University of California Davis, Davis, CA; ²Lung Center of the Philippines, Quezon City, Philippines; ³University of the Philippines Los Baños, Los Baños, Philippines**
- TP 300 **Altered N-Glycoproteome of Murine Keratinocyte-Originated Exosomes under Diabetic Conditions Compromised Resolution of Wound Inflammation; Xuyao Zeng¹; Adam J Anthony¹; Anu Sharma²; Jonathan C. Trinidad¹; Subhadip Ghatak²; David E. Clemmer¹; ¹Indiana University Bloomington, Bloomington, IN; ²Indiana University Purdue University Indianapolis, Indianapolis, IN**
- TP 301 **Sialic acid isomer-targeted glycoprotein enrichment and proteomic characterization using bioorthogonal derivatization; Hongxia Bai¹; Collin McDowell¹; Richard R. Drake¹; ¹Medical University of South Carolina, Charleston, SC**
- TP 302 **Mass Spectrometry Analysis of N-linked Glycosylation on Influenza A(H3N2) Hemagglutinin and**

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- TP 303 **Neuraminidase from Inactivated Virus; Betlehem Mekonnen¹; Irina Alymova²; Jakub Baudys¹; Ian York²; Donxia Wang¹; John R Barr¹; ¹CDC, Chamblee, GA; ²CDC, Atlanta, GA**
- TP 304 **Confident Identification of Multiply Glycosylated Peptides Using Hot Electron Capture Dissociation; Margaret Downs¹; Cheng Lin¹; Chaoshuang Xia¹; Athanasios Smyrnakis²; Dimitris Papanastasiou²; Joseph Zaia¹; ¹Boston University Chobanian and Avedisian School of Medicine, Boston, MA; ²Fasmatech, NCSR Demokritos, Athens, Greece**
- TP 305 **Comparative Glycomic and Glycoproteomic Analysis of Serum Exosomes Isolated Using Ultracentrifugation and Affinity-Based Method; Mojibola O Fowowe¹; Cristian D Gutierrez-Reyes¹; Mojgan Atashi¹; Sherifdeen Onigbinde¹; Judith Nwaiwu¹; Oluwatosin E Daramola¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX**
- TP 306 **O-glycoproteomic mapping of amyloid precursor protein in Alzheimer's Disease; Alexandria S. Battison¹; Stacy A. Malaker¹; ¹Yale University, New Haven, CT**
- TP 307 **Target Glycoproteomics and Proteomics Analysis with Parallel Reaction Monitoring (PRM) LC-MS/MS; Moyinoluwa A Adeniyi¹; Cristian D Gutierrez Reyes¹; Mojgan Atashi¹; Andrew I Bennett¹; Sherifdeen Onigbinde¹; Rogelio Najera Gonzalez²; David M Lubman³; Yehia Mechref¹; ¹Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; ²Institute of Genomics for Crop Abiotic Stress Tolerance, Texas Tech University, Lubbock, TX; ³Department of Surgery, The University of Michigan, Ann Arbor, MI**
- TP 308 **The role of N-glycosylation in SARS-CoV-2 Spike protein binding specificity and kinetics; Sarah H Osman¹; Dongxia Wang¹; Theodore R. Keppel¹; John R Barr¹; ¹CDC, Chamblee, GA**
- TP 309 **Isomeric Separation of $\alpha 2,3/\alpha 2,6$ -linked 2-aminobenzamide (2AB)-labeled Sialoglycopeptides by C18-LC-MS/MS; Peilin Jiang¹; Yifan Huang¹; Cristian D Gutierrez Reyes¹; Jieqiang Zhong¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, Texas**
- TP 310 **Analysis of Mitochondria Glycomics and Glycoproteomics Isolated Using Different Enrichment Methods; Judith Ijeoma Nwaiwu¹; Oluwatosin E Daramola¹; Mojgan Atashi¹; Mojibola O Fowowe¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, Texas**
- TP 311 **LC-MS/MS Characterization of the N-glycosylation of Spike protein S1 Derived from 11 variants of SARS-CoV-2; Cristian D Gutierrez Reyes¹; Sherifdeen Onigbinde¹; Andrew I. Bennett¹; Akeem Sanni¹; Peilin Jiang¹; Oluwatosin E Daramola¹; Mojgan Atashi¹; Vishal Sandilya¹; Mojibola O Fowowe¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, Texas**
- TP 312 **Improved enrichment techniques for analysis of densely O-glycosylated domains from complex samples; Keira Erol Mahoney¹; Vincent Chang¹; Taryn M. Lucas¹; Stacy A. Malaker¹; ¹Yale University, New Haven, CT**
- TP 313 **Comparison of the Relative Quantitation of N-linked Glycopeptides Using Different Chromatographic Separation Modes; Mya M Brown¹; Hoang Kim Ngan Thai¹; Ron Orlando¹; ¹University of Georgia - Complex Carbohydrate Research Center, Athens, GA**
- TP 314 **Development of an Automatic Three-Dimensional Mass Spectrometry Imaging System with Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI); Ying Xi¹; Kevan Knizner¹; Kenneth Garrard¹; David Muddiman¹; ¹North Carolina State University, Raleigh, NC**
- TP 315 **Achieving Sub Parts-Per-Million Mass Measurement Accuracy on an Orbitrap Mass Spectrometry Imaging Platform without Automatic Gain Control; Russell R. Kibbe¹; David C. Muddiman¹; ¹North Carolina State University, Raleigh, NC**
- TP 316 **Super-resolution Expansion Mass Spectrometry Imaging; Y. L. Winnie Hung¹; Jianing Wang¹; Chengyi Xie¹; Zongwei Cai¹; ¹State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, China**
- TP 317 **A simplified sample preparation strategy for high-throughput mass spectrometry imaging of spheroids; Yuan Liu¹; Jillian Johnson¹; Hua Zhang¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI**
- TP 318 **immuno-DESI-MSI Spatially Locates A Drug Target, Signaling Factors, and Enzymes on Tissue; Xiaowei Song¹; Richard N. Zare¹; ¹Stanford University, Stanford, CA**
- TP 319 **Quantitative Biodistributions of Polymeric Nanocarriers and their Cargo via Metal-coded Mass Tag Approach; Dheeraj K. Agrohia¹; Ritabrita Goswami¹; Teerapong Jantararat¹; Yağız Anil Çiçek¹; Taewon Jeon¹; Vincent M. Rotello¹; Richard W. Vachet¹; ¹University of Massachusetts, Amherst, AMHERST, MA**
- TP 320 **Improved Quantitative Imaging of Nanomaterials by LA-ICP-MS using a Novel Tissue Mimic Approach; Teerapong Jantararat¹; Joshua D Lauterbach¹; Jeerapat Douchchawee¹; Richard W. Vachet¹; ¹University of Massachusetts Amherst, Amherst, MA**
- TP 321 **RaMALDI imaging: a novel multimodal imaging workflow integrating Raman spectroscopic and MALDI mass spectrometry imaging of a single sample; Jeong Hee Kim¹; Ethan Yang²; Caitlin M Tressler²; Xinyi Elaine Shen²; Dalton R Brown²; Cole Johnson²; Ishan Barman¹; Kristine Glunde²; ¹Johns Hopkins University, Baltimore, MD; ²Johns Hopkins University School of Medicine, Baltimore, MD**
- TP 322 **Statistical Approach to System Suitability Testing (SST) for Mass Spectrometry Imaging by Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI); Olivia Dioli¹; Hongxia Bai¹; Emily Hector¹; Kenneth P Garrard¹; David C Muddiman¹; ¹North Carolina State University, Raleigh, NC**
- TP 323 **Combining Multimodal Single Cell Imaging with Multiplexed Enzyme-based MALDI Mass Spectrometry Imaging for Translational Studies; Jaclyn B Dunne¹; Jake T. Griner¹; Martin Romeo¹; Carsten Krieg¹; Mark Lim²; Anand S. Mehta¹; Richard R. Drake¹; Peggy M. Angel¹; ¹Medical University of South Carolina, Charleston, SC; ²AmberGen, Inc., Billerica, MA**
- TP 324 **Visualizing the Matrix: New Methods for Imaging the Distributions of Extracellular Matrix Proteins; Akaansha Rampal¹; Ngoc Vu¹; Richard W. Vachet¹; Shelly R. Peyton¹; ¹University of Massachusetts Amherst, Amherst, MA**
- TP 325 **High-coverage lipid C=C location isomers mass spectrometry imaging in biological tissues and tumor model; Yanyan Chen¹; Chengyi Xie¹; Peisi Xie¹; Jianing Wang¹; Zongwei Cai¹; ¹State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, China**
- TP 326 **Tissue treatment and post-ionization for mass spectrometry imaging of lipids: gains and losses; Junhai Yang¹; Austin B. Moyle¹; Andrew Bowman¹; Wayne Buck¹; David S. Wagner¹; ¹AbbVie Inc., North Chicago, IL**
- TP 327 **Robust tissue single-voxel collection and processing for spatially resolved proteomics; Reta Birhanu Kitata¹; Marija Velickovic²; Zhangyang Xu¹; Rui Zhao³; Rosalie K. Chu⁴; Marda L. Jorgensen⁴; David Scholten⁵; Tao Liu¹; Huiping Liu⁵; Clive H. Wasserfall⁴; Chia-Feng Tsai¹; Tujin Shi¹; ¹Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington 99354; ²Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; ³Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; ⁴Department of Pathology, Immunology, and Laboratory Medicine, Diabetes Institute, College of Medicine, University of Florida, Gainesville, Florida 32611;**

TUESDAY POSTERS

- ⁵*Department of Pharmacology, Feinberg School of Medicine, Northwestern University, Chicago, Illinois 60611*
- TP 327 **A Tailored Approach for the Analysis of Membrane Proteins from Tissue by Native Nano-DESI Mass Spectrometry**; Emma K. Sisley¹; Oliver J. Hale¹; Helen J. Cooper¹; ¹*University of Birmingham, Birmingham, United Kingdom*
- TP 328 **MALDI coupled with 193 nm ultraviolet photodissociation for the characterization of glycerophospholipids**; Melanie J Campbell¹; Erin H. Seeley¹; Jennifer S. Brodbelt¹; ¹*University of Texas at Austin, Austin, TX*
- TP 329 **Multimodal mass spectrometry imaging to elucidate the mechanisms of ferroptosis in epithelial ovarian cancer**; Brittney L Gorman¹; Michael Taylor¹; Lia Tesfay²; Jessica K Lukowski¹; Suzy Torti²; Christopher Anderton¹; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*Department of Molecular Biology and Biophysics, University of Connecticut Health Center, Farmington, CT*
- TP 330 **Biofilm of pathogenic bacteria analyzed by MALDI-TOF imaging mass spectrometry (IMS) and top-down proteomic identification**; Clifton K Fagerquist¹; Yanlin Shi¹; ¹*Produce Safety & Microbiology, Western Regional Research Center, Agricultural Research Service, USDA, Albany, CA*
- TP 331 **4-APEBA, a new on-tissue chemical derivatization agent for enhanced imaging of phytochemicals using MALDI-MSI**; Kevin J Zemaitis¹; Vivian Lin¹; Amirhossein H. Ahkami¹; Tanya Winkler¹; Robert Stanley¹; Vimal Kumar Balasubramanian¹; Christopher Anderton¹; Dusan Velickovic¹; ¹*PNNL, Richland, WA*
- TP 332 **SpatialOMx analysis allows for the specific identification of lipid species paving the way for accurate flux analysis**; Sumankalai Ramachandran¹; Beixi Wang¹; Azad Eshghi¹; Erica Forsberg¹; Katherine Stumpo¹; ¹*Bruker Daltonics, Billerica, MA*
- TP 333 **MALDI-IHC-Guided In-Depth Spatial Proteomics: Targeted and Untargeted MSI Combined**; Britt S.R. Claes¹; Kasper Krestensen¹; Gargey Yagnik²; Andrej Grgic¹; Christel Kuik¹; Mark J. Lim²; Kenneth J. Rothschild²; Michiel Vandenbosch¹; Ron M.a. Heeren¹; ¹*Maastricht MultiModal Molecular Imaging Institute, Maastricht University, Maastricht, Netherlands*; ²*AmberGen, Inc., Billerica, MA*
- TP 334 **Maximizing Throughput of a Liquid Microjunction-Surface Sampling Probe-Mass Spectrometry Imaging System for Microfluidic Rhizosphere-on-a-Chip Habitats**; Vilmos Kertesz¹; Scott T. Retterer¹; Muneeba Khalid¹; John F. Cahill¹; ¹*Oak Ridge National Laboratory, Oak Ridge, TN*
- TP 335 **Mass spectrometry imaging of regioisomeric hormonal steroids**; Varun Vashneel Sharma¹; Ingela Lanekoff²; ¹*Uppsala University, Uppsala, Sweden*; ²*Uppsala University, Uppsala, Sweden*
- TP 336 **Functionality of Sucrose as a Cryoprotectant and Permeative Matrix for Analysis of Multiple Biological Systems by IR-MALDESI Mass Spectrometry Imaging**; Mary F Wang¹; Alexandria L. Sohn¹; Juhi Samal²; Kevin Erning²; Tatiana Segura²; David C. Muddiman¹; ¹*North Carolina State University, Raleigh, NC*; ²*Duke University, Durham, NC*
- TP 337 **Image-wide adjacent-pixel data averaging increases sensitivity toward dosed drugs of abuse and antiretrovirals in Q Exactive mass spectrometry imaging**; Yury N. Desyaterik¹; Austin M. Jones²; Kara M. Rademeyer²; Mary Peace McRae²; Yury O. Tsybin³; Konstantin O. Nagornov³; Anton N. Kozhinov³; Angela D.M. Kashuba¹; Elias P. Rosen¹; ¹*UNC, Chapel Hill, NC*; ²*Virginia Commonwealth University, Richmond, VA*; ³*Spectroswiss, Lausanne, Switzerland*
- TP 338 **Improved detection of tryptic peptides from tissue sections using Desorption electrospray ionisation mass spectrometry imaging (DESI-MSI)**; Heather Bottomley¹; Dr Jonathan Phillips¹; Dr Philippa Hart²; ¹*University of Exeter, Exeter, United Kingdom*; ²*Medicines Discovery Catapult, Manchester, United Kingdom*
- TP 339 **Evaluation of lithium adduction in mass spectrometry imaging for sphingolipid analysis via internal standard-spiked tissue homogenate**; Anh Tran¹; William T. Andrews¹; Eugene Moskovets²; Maureen A. Kane¹; Jace W. Jones¹; ¹*University of Maryland, School of Pharmacy, Baltimore, MD*; ²*Mass Tech Inc., Columbia, Maryland*
- TP 340 **AutoPiMS: an Integrated Mass Spectrometry Imaging Workflow for Spatial Proteoform Biology**; Pei Su¹; John P. McGee¹; Kenneth R Durbin¹; Michael A. R. Hollas¹; Thomas P. Conrads²; Ryan T. Fellers¹; Jeannie M. Camarillo¹; Jared O. Kafader¹; Neil L. Kelleher¹; ¹*Northwestern University, Evanston, IL*; ²*Women's Health Integrated Research Center at Inova Health System, Annandale, VA*
- TP 341 **Spatial Proteomics Reveals Localization of Membrane Proteins and Post-Translational Modifications in Ocular Lenses**; Kevin L. Schey¹; Lee S Cantrell²; Zhen Wang¹; ¹*Vanderbilt University, Department of Biochemistry, Nashville, TN*; ²*Vanderbilt University, Nashville, TN*
- TP 342 **Art Conservation with DESI MS Imaging: Direct Mapping of Compound Localization on Wood Samples**; Luke Addington¹; Michael T Marty¹; Anthony J Midey²; ¹*University of Arizona, Tuscon, Arizona*; ²*Waters, Milford, MA*
- TP 343 **Spatial molecular analysis of acute cocaine exposure**; Mariya Nezhyva¹; Rami Yaka²; Per E. Andr'en¹; Katy Margulis²; Erik T Jansson¹; ¹*Uppsala University, Uppsala, Sweden*; ²*Hebrew University, Jerusalem, Israel*
- TP 344 **Evolution from Shotgun to Machine-gun - Capillary LC/MS with 1,000 Samples/Day Facilitates Proteomic MS Imaging**; Ayana Tomioka¹; Ryota Tomioka¹; Kosuke Ogata¹; Issei Mori^{2,3}; Makoto Arita^{2,3}; Koshi Imami²; Naoyuki Sugiyama¹; Yasushi Ishihama^{1,4}; ¹*Kyoto University, Kyoto, Japan*; ²*RIKEN Center for Integrative Medical Sciences, Yokohama, Japan*; ³*Keio University, Minato-ku, Japan*; ⁴*National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan*
- TP 345 **Evaluation of an improved feature finding algorithm for QTOF and ion mobility imaging data in spatial lipidomics and metabolomics**; Jacob Truong^{1,2,3}; Sören-Oliver Deininger⁴; Andra Pascale-Henke⁴; Konstantin Schwarze⁴; Lisa M. Butler^{1,2,3}; Paul J. Trim^{1,3}; Marten F. Snel^{1,3}; Heiko Neuweger⁴; ¹*University of Adelaide Medical School and Freemasons Centre for Male Health and Well-being, Adelaide, Australia*; ²*South Australian Immunogenomics Cancer Institute, Adelaide, Australia*; ³*South Australian Health and Medical Research Institute, Adelaide, Australia*; ⁴*Bruker Daltonics GmbH & Co. KG, Bremen, Germany*
- TP 346 **Exudate Dynamics of the Rhizosphere Visualized Using MALDI-MSI**; Fiona M Ellsworth¹; Joshua L Fischer²; Ethan Yang²; Kasia Janota²; Richard E. Marinos¹; ¹*University at Buffalo, Buffalo, NY*; ²*Bruker Daltonics, Billerica, MA*
- TP 347 **Exploring the Potential of Mass Spectrometry Imaging: Opportunities and Challenges**; Michaela Schwaiger-Haber¹; Ethan Stancliffe¹; Dhanalakshmi S. Anbukumar¹; Blake E. Sells¹; Jia Yi¹; Kevin Cho¹; Kayla Adkins-Travis¹; Leah P. Shriver¹; Gary J. Patti¹; ¹*Washington University in St. Louis, St. Louis, MO*
- TP 348 **2D (phospho-)proteome mapping of human spleen tissue at 200 µm spatial resolution**; Marija Velickovic^{#1}; Reta Birhanu Kitata^{#1}; Zhangyang Xu¹; Rui Zhao¹; Rosalie K. Chu¹; Marda L. Jorgensen²; David Scholten³; Sarah M Williams¹; Ying Zhu¹; Daniel J Orton¹; Tao Liu¹; Huiping Liu³; Clive H. Wasserfall²; Chia-Feng Tsai¹; Tujin Shi¹; ¹*PNNL, Richland, WA*; ²*University of Florida, Gainesville, FL*; ³*Department of Pharmacology, Feinberg School of Medicine, Northwestern University, Chicago, Illinois 60611*

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- TP 349 **Using Native MS, Top-Down, and Bottom-Up Proteomics to Profile Regio-specific Protein Interactions on Tissue;** Sarah C Beno¹; Raul A Villacob¹; Neda Feizi Gilandeh¹; Touradj Solouki¹; ¹Baylor University, Waco, TX
- TP 350 **Spatial Multi-Omics Investigation of Prostate Cancer Heterogeneity using integrated spatially resolved lipidomics and transcriptomics;** Wangju Zhang^{1,2}; Xander Spotbeen³; Tassiani Sarretto^{4,5}; Fabio Socciarelli⁶; Sebastiaan Vanuytven^{7,8}; Jose Ignacio Alvira Larizgoitia^{9,10}; Sam Kint^{7,9}; David Wouters^{9,11}; Gabriele Partel⁹; Maria Mantas¹²; Thomas Gevaert¹³; Wout Devlies^{14,15}; Katy Vandereyken^{7,9}; Steven Joniau^{14,16}; Massimo Loda¹⁷; Bart De Moor¹⁸; Thierry Voet^{7,9}; Alejandro Sifrim^{9,11}; Shane Ellis^{5,19}; Marc Claesen¹²; Nico Verbeeck¹²; Johannes Swinnen²⁰; ¹STADIUS Center for Dynamical Systems, Signal Processing and Data Analytics, Department of Electrical Engineering (ESAT), KU Leuven, Leuven, Belgium; ²Aspect Analytics NV, Genk, Belgium; ³Laboratory of Lipid Metabolism and Cancer, KU Leuven and Leuven Cancer Institute (LKI), Leuven, Belgium; ⁴Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; ⁵Illawarra Health and Medical Research Institute, Wollongong, Australia; ⁶Department of Pathology, Weill Cornell Medical College, New York, NY; ⁷Laboratory of Reproductive Genomics, Department of Human Genetics, KU Leuven, Leuven, Belgium; ⁸KU Leuven Institute for Single Cell Omics (LISCO), KU Leuven, Leuven, Belgium; ⁹KU Leuven Institute for Single Cell Omics (LISCO), KU Leuven, Leuven, Belgium; ¹⁰Laboratory of Multi-omic Integrative Bioinformatics, Department of Human Genetics, KU Leuven, Leuven, Belgium; ¹¹Laboratory of Multi-omic Integrative Bioinformatics, Department of Human Genetics, KU Leuven, Leuven, Belgium; ¹²Aspect Analytics NV, Genk, Belgium; ¹³Department of Urology, University Hospitals Leuven, Leuven, Belgium; ¹⁴Department of Urology, University Hospitals Leuven, Leuven, Belgium; ¹⁵Department of Development and Regeneration, KU Leuven, Leuven, Belgium; ¹⁶Department of Development and Regeneration, KU Leuven, Leuven, Belgium; ¹⁷Department of Pathology, Weill Cornell Medical College, New York, New York; ¹⁸STADIUS Center for Dynamical Systems, Signal Processing and Data Analytics, Department of Electrical Engineering (ESAT), KU Leuven, Leuven, Belgium; ¹⁹Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; ²⁰Laboratory of Lipid Metabolism and Cancer, KU Leuven and Leuven Cancer Institute (LKI), Leuven, Belgium
- TP 351 **Lipid Annotation for MALDI Imaging using Isotope Pattern, Spectral Pattern and Co-Localization Information;** Jeff Dahl¹; Md Amir Hossen²; ¹Shimadzu, Columbia, MD; ²Shimadzu Scientific Instrument, Columbia, Maryland
- TP 352 **Development of Robust Spatial N-Glycomics and Proteomics Techniques for Human Tissue Analysis;** Jessica K Lukowski^{1,2}; Connor West³; Katherine A. Stumpo³; Young Ah Goo^{1,2}; ¹Mass Spectrometry Technology Access Center (MTAC@MGI), St Louis, MO; ²Washington University School of Medicine, St. Louis, MO; ³Bruker Daltonics GmbH & Co.KG, Bremen, Germany
- TP 353 **Single-voxel spatial proteomics for resolving 14 ROIs across the whole mouse brain tissue section;** Zhangyang Xu¹; Reta Birhanu Kitata¹; Rosalie K. Chu¹; Rui Zhao²; Le Z. Day¹; Matthew J Gaffrey¹; Tao Liu¹; Song-Lin Ding³; Tong Zhang¹; Tujin Shi¹; ¹Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington 99354; ²Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; ³Allen Institute for Brain Science, Seattle, Washington 99354
- TP 354 **Characterizing Molecular Alterations to Glomeruli in Diabetic Nephropathy using MALDI IMS, Immunohistochemistry;** Angela RS Kruse^{1,2}; Melissa A Farrow^{1,2}; Nathan Heath Patterson^{1,2}; Madeline Colley^{1,2}; Jamie L Allen^{1,2}; Roy Lardenoije³; Lukasz G Migas⁴; Morad Malek^{1,5}; Haichun Yang^{6,7}; Agnes B Fogo^{6,7,8}; Raf Van De Plas^{1,2,4}; Joana P Goncalves³; Richard M Caprioli^{1,2,9,10,11}; Jeffrey M Spraggins^{1,2,5,11}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Biochemistry, Vanderbilt University, Nashville, TN; ³Department of Intelligent Systems, Delft University of Technology, Delft, South Holland; ⁴Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ⁵Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; ⁶Department of Pathology, Microbiology and immunology, Vanderbilt University, Nashville, TN; ⁷Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; ⁸Division of Nephrology, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; ⁹Department of Medicine, Vanderbilt University, Nashville, TN; ¹⁰Department of Pharmacology, Vanderbilt University, Nashville, TN; ¹¹Department of Chemistry, Vanderbilt University, Nashville, TN
- TP 355 **Maximizing Data Coverage with Sequential Imaging of a Single Tissue Section;** Erin H Seeley¹; Edwin Escobar¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- TP 356 **Bridging the Spatial Gap: A Method Enabling Spatial Transcriptomics and Lipidomics Within the Same Tissue Section;** Morad C Malek^{1,2}; Martin Dufresne^{1,3}; Angela RS Kruse^{1,3}; Christopher J Good^{1,4}; Roy Lardenoije⁵; Lukasz G Migas^{1,6}; Melissa A Farrow^{1,3}; Katerina V Djambazova^{1,2}; Jamie L Allen^{1,3}; Raf Van De Plas^{1,3,6}; Joana P Goncalves⁵; Jeffrey M Spraggins^{1,2,3,4}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Department of Chemistry, Vanderbilt University, Nashville, TN; ⁵Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands; ⁶Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands
- TP 357 **Spatial metabolomics via MALDI-MSI identifies pharmacodynamic biomarkers for diabetic kidney disease;** Leila Hejazi^{1,2}; Guanshi Zhang²; Shoba Sharma¹; Aaron Ruiz¹; Fabio C Tucci³; Kumar Sharma²; ¹SygnMap, Inc., San Antonio, TX; ²Center for Precision Medicine, UT Health San Antonio, San Antonio, Texas; ³Epigen Biosciences, San Diego, CA
- TP 358 **In-situ N-glycosylation signatures of ovarian cancer deciphered by combination of multimodal MS imaging and LC-MS/MS;** Penghsuan Huang¹; Hua Zhang²; Manish Patankar³; Lingjun Li^{1,2}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ³Department of Obstetrics and Gynecology, University of Wisconsin-Madison, Madison, WI
- TP 359 **The development of Expansion Mass Spectrometry (EXMS) towards studying spatial single cell metabolomics;** Sarah E Levy¹; Vignesh Venkataramani²; Laura Sanchez³; Lydia Kislely²; ¹University of California Santa Cruz, Santa Cruz, CA; ²Department of Biophysics and Chemistry, Case Western Reserve University, Cleveland, OH; ³University of California, Santa Cruz, Santa Cruz, CA
- TP 360 **Updates to FragPipe computational platform: new capabilities, tools, and workflows;** Fengchao Yu¹; Daniel Polasky¹; Guo Ci Teo¹; Felipe Da Veiga Leprevost¹; Kai Li¹; Kevin L Yang¹; Yi Hsiao¹; Ginny Xiaohe Li¹; Carolina Rojas Ramirez¹; Sarah Haynes¹; Daniel J Geiszler¹; Hui-Yin

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- Chang^{1,2}; Dmitry Avtonomov¹; Andy T. Kong¹; Alexey I Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI; ²National Central University, Taoyuan, Taiwan
- TP 361 **Localized Microsampling of Formalin Fixed Paraffin Embedded Tissue for Proteomics**; Blessing Chisom Egbejiogu¹; Kermit K. Murray¹; ¹Louisiana State University, Baton Rouge, LA
- TP 362 **Development of an Easy-to-use Python Script for Visualizing Deconvoluted Top-Down Mass Spectrometric Data: A Histone Case Study**; Megan Bindra¹; Udayan Das¹; James Pesavento¹; ¹Saint Mary's College, Moraga, CA
- TP 363 **Characterization of proteoform post-translational modifications by top-down and bottom-up mass spectrometry and UniProt annotations**; Wenrong Chen¹; Yong Zang²; Xiaowen Liu^{3,4}; ¹Department of BioHealth Informatics, Indiana University-Purdue University Indianapolis, Indianapolis, IN; ²Department of Biostatistics and Health Data Sciences, Indiana University School of Medicine, Indianapolis, IN; ³Deming Department of Medicine, Tulane University, New Orleans, LA; ⁴Tulane Center for Biomedical Informatics and Genomics, Tulane University, New Orleans, LA
- TP 364 **TMT complementary ion-based interference removal enables accurate quantification for 18-plex proteomics**; Yingxue Fu¹; Huan Sun¹; Zhiping Wu¹; Zhen Wang¹; Suresh Poudel¹; Zuo-Fei Yuan¹; Karthik Vadambacheri Manian¹; Xusheng Wang¹; Junmin Peng¹; ¹St. Jude Children's Research Hospital, Memphis, TN
- TP 365 **Optimization of DIA proteomics workflows using ground truth data simulated with Synthedia**; Michael G Leeming¹; Ching-Seng Ang¹; Shuai Nie¹; Swati Varshney¹; Nicholas A Williamson¹; ¹The University of Melbourne, Melbourne, Australia
- TP 366 **Highly sensitive and scalable timsTOF Pro data analysis with MaxDIA 2.0**; Juan L Restrepo-López¹; Dmitry Alexeev¹; Carlo De Nart¹; Juergen Cox¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany
- TP 367 **FilterFASTA: a Tool for Generating Keyword Based Bespoke Cross-Organism FASTA's for Proteomics**; John Chlystek¹; Jonathan Le¹; Jonathan Katz^{1,2}; ¹Lawrence J. Ellison Institute for Transformative Medicine, Los Angeles, CA; ²USC, Los Angeles, CA
- TP 368 **An adaptive model for the protein inference problem**; Emile Benoist¹; Guillaume Fertin¹; Géraldine Jean¹; ¹LS2N, Nantes Université, Nantes Cedex 3, France
- TP 369 **Bayesian Confidence Intervals for Absolute Protein Quantification**; Chirag K Kumar¹; Meera Gupta¹; Donovan Cassidy-Nolan¹; Arjuna Subramanian¹; Vyas Pujari¹; Martin Wuehr¹; ¹Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ
- TP 370 **The Challenge of Plant Identification in Complex Mixtures: Closely Related Families, Large Proteomes, and Unsequenced Genomes**; Melinda A. McFarland¹; Sara M. Handy¹; Elizabeth Hunter¹; Christine H. Parker¹; Ann M. Knolhoff¹; ¹FDA-CFSAN, College Park, MD
- TP 371 **A Streamlined Data Analysis Workflow for Enhanced New Peak Detection (NPD) in the Multi-Attribute Method (MAM)**; Maurizio Bronzetti¹; Aude Tartiere¹; Stephen Kok¹; Amy Claydon²; Arnd Brandenburg³; ¹Genedata Inc., San Francisco, CA; ²Genedata Ltd, Cambridge, United Kingdom; ³Genedata AG, Basel, Switzerland
- TP 372 **PyC2MC: an open-source software solution for visualization and treatment of high-resolution mass spectrometry data**; Maxime Sueur^{1,2}; Julien Maillard^{1,2,3}; Oscar LACROIX-ANDRIVET^{1,2,4}; Christopher Rueger^{2,5}; Pierre Giusti^{1,2,3}; Hélène Lavanant¹; Carlos Afonso^{1,2}; ¹Normandie Univ, UNIROUEN, INSA Rouen, CNRS, COBRA, 76000 Rouen, France., Mont Saint Aignan, France; ²International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harfleur, France; ³TotalEnergies OneTech R&D, TotalEnergies Research & Technology, Gonfreville, France; ⁴TotalEnergies Marketing Services, Research Center, Solaize, France; ⁵Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany
- TP 373 **MS-based identification of the mutated peptides in HCT116 cell line through searching against a SNVs dataset derived from integrated transcriptomes**; Xia Zhang^{1,2}; Jiawei Liu²; Yabing Zhu³; Zhe Ren²; Siqi Liu^{1,2}; ¹College of Life Science, University of Chinese Academy of Sciences, Beijing, China; ²Center of Proteomic Analysis, BGI Life Science Research Institute, Shenzhen, China; ³BGI Genomics, BGIShenzhen, Shenzhen, China
- TP 374 **Fast Component Identification & Automated Well-to-Data Connectivity for High Throughput Workflows**; Richard Lee¹; Nikki Dare¹; Rostislav Pol¹; Sofya Chudova¹; Nikolay Malashchenok¹; ¹ACD/Labs, Toronto, ON
- TP 375 **Streamlining Metadata Capture for Mass Spectrometry Experiments: towards FAIR Omics metadata across R&D**; Benjamin Pullman¹; Norelle C. Wildburger¹; Matthew Glover¹; Raghothama Chaerkady¹; Jana Zecha¹; Sri Vishnu Vardhan Deevi²; Lisa H Cazares¹; Sonja Hess¹; Stewart MacArthur²; Sebastian Wasilewski²; ¹AstraZeneca, Gaithersburg, MD; ²AstraZeneca, Cambridge, United Kingdom
- TP 376 **Creating a data analysis pipeline for producing high-quality glycopeptide mass spectral libraries**; Sergey Sheetlin¹; Yuri A. Mirokhin¹; Guanghui Wang¹; Xiaoyu Yang¹; Concepcion Remorosa¹; Yi Liu¹; Xinjian Yan¹; Dmitrii V. Tchekhovskoi¹; Zachary C. Goecker¹; Meghan C. Burke¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD
- TP 377 **Prohits 8.0: MS2-based quantitative workflow to improve sensitivity and quantitative accuracy of proximity-dependent biotinylation experiments**; Shubham Gupta^{1,2}; Guomin Liu³; Brett Larsen³; Geoffrey Hesketh⁴; Payman Samavarchi Tehrani³; Hala Abdouni³; Anne-Claude Gingras^{1,3}; Hannes Röst^{1,2}; ¹University of Toronto, Toronto, ON; ²Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON; ³Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto, ON; ⁴Dalhousie University, Halifax, NS
- TP 378 **Workflomics: Facilitating the "Great Bake Off" of Computational Workflows for the Analysis of Mass Spectrometry Data**; Vedran Kasalica¹; Nauman Ahmed¹; Rob J Marissen²; Saskia Hiltmann³; Pratik Jagtap⁴; Melanie Föll⁵; Hervé Ménager⁶; Matúš Kaláš⁷; Michael R. Crusoe^{8,9}; Ana Redondo¹⁰; Salvador Capella-Gutierrez¹⁰; Veit Schwämmle¹¹; Anna-Lena Lamprecht¹²; Magnus Palmblad²; ¹Netherlands eScience Center, Amsterdam, Netherlands; ²Leiden University Medical Center, Leiden, Netherlands; ³Erasmus Medical Center Rotterdam, Rotterdam, Netherlands; ⁴University of Minnesota, Minneapolis, MN; ⁵University of Freiburg, Freiburg, Germany; ⁶Institute Pasteur, Paris, France; ⁷University of Bergen, Bergen, Norway; ⁸Vrije Universiteit Amsterdam, Amsterdam, Netherlands; ⁹Forschungszentrum Jülich, Jülich, Germany; ¹⁰Barcelona Supercomputing Center, Barcelona, Spain; ¹¹University of Southern Denmark, Odense, Denmark; ¹²University of Potsdam, Potsdam, Germany
- TP 379 **MassKit: A Flexible and High Performance API for Mass Spectrometry**; Douglas Slotta¹; Lewis Y. Geer¹; ¹NIST, Gaithersburg, MD
- TP 380 **Chimersy server: deploying the power of the cloud in your basement**; Markus Schneider¹; Tobias Schmidt¹; Daniel P. Zolg¹; Siegfried Gessulat¹; Florian Seefried¹; Samia Ben Fredj¹; Martin Heinrich Frejno¹; ¹MSAID GmbH, Garching b.München, Germany
- TP 381 **Data - Information - Knowledge effortlessly: Combining timsTOF data with PaSER information and Mass Dynamics knowledge to accelerate proteomic discoveries**; Tharan Srikumar¹; Mark Rocco Condina²;

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- Jonathan Krieger¹; Giuseppe Infusini²; Brad Green²; Paula Burton Ngov²; Aaron Triantafyllidis²; Saima Ahmed^{3,4}; Arthur Viode^{3,4}; Patrick Van Zalm^{3,4}; Sven Brehmer⁵; Dennis Trede⁵; Christopher Adams⁶; Judith Steen^{3,4}; Shibani S. Mukerji⁴; Hanno Steen^{3,4}; Andrew Ian Webb²; ¹Bruker Ltd., Milton, ON; ²Mass Dynamics, Melbourne, Australia; ³Boston Childrens Hospital, Boston, MA; ⁴Harvard Medical School, Boston, MA; ⁵Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ⁶Bruker Scientific, San Jose, CA
- TP 382 **prolfquapp: Streamlining Protein Differential Expression Analysis in Core Facilities**; Witold E. Wolski¹; Jonas Grossmann¹; Paolo Nanni¹; Bernd Roschitzki¹; Claudia Fortes¹; Christian Panse¹; Ralph Schlapbach¹; ¹Functional Genomics Center Zurich, University of Zurich & ETH Zurich, Zurich, Switzerland
- TP 383 **A semi-automated workflow for DIA-based global discovery to pathway-driven PRM analysis on a TIMS-QTOF instrument**; Jennifer Guergues¹; Jonathan R Krieger²; John M Koomen³; Sameer Varma¹; Stanley Stevens Jr.¹; ¹University of South Florida, Tampa, FL; ²Bruker Ltd., Milton, ON; ³Moffitt Cancer Center, Tampa, FL
- TP 384 **Sample to Result Workflow for the Investigation of Biosimilars vs Innovator Cetuximab by Charge Variant Analysis using Microchip CE-MS**; Antony Harvey¹; Adi M Kulkarni²; Kristina Srzentic³; Marshall Bern¹; Ignat Shilov¹; St. John Skilton¹; Kate Yu²; ¹Protein Metrics, LLC, Cupertino, CA; ²908 Devices, Inc., Boston, MA; ³ThermoFisher Scientific, San Jose, CA
- TP 385 **Tidyproteomics: An open-source R package and data object for quantitative proteomics post analysis and visualization**; Jeffrey J. Jones¹; Brett Lomenick¹; Ting-You Wang¹; Tsui-Fen Chou¹; ¹Caltech, Pasadena, CA
- TP 386 **Centralized metabolomics reference database for standardized small molecule mass spectrometry data analysis**; Anastasiya V. Prymolenna¹; Jordan M. Rabus¹; Montana L. Smith¹; Natasha N. Arokium-Christian¹; Priscila M. Lalli¹; Chaevien S. Clendinen¹; Nathalie Munoz Munoz¹; William R. Kew¹; Young-Mo Kim¹; Lee Ann McCrue¹; Yuri E. Corilo¹; ¹Pacific Northwest National Laboratory, Richland, WA
- TP 387 **MiCId GUI, a fast Microorganism Classification and Identification workflow with accurate statistics and high recall**; Aleksey Y Ogurtsov¹; Gelio Alves¹; Yi-Kuo Yu¹; ¹CBB NCBI NLM NIH, Bethesda, MD
- TP 388 **Open Platform for Automated Backup, Processing and Visualization of MS-based Omics Data**; Xiaofeng Xie¹; Thy Truong¹; Kei Webber¹; Yiran Liang¹; Madisyn Johnston¹; Samuel H Payne¹; Ryan Kelly¹; ¹Brigham Young University, Provo, UT
- TP 389 **MassIVE: adding value to all public data through automatic indexing and query tools**; Jeremy Carver¹; Nuno Bandeira¹; ¹UCSD, La Jolla, CA
- TP 390 **Proteomics Standards Initiative (PSI) proposed peak annotation format (mzPAF) and spectral library format (mzSpecLib) standards**; Henry Lam¹; Tytus D. Mak²; Joshua A. Klein³; Wout Bittremieux⁴; Ralf Gabriels⁵; Yasset Perez-Riverol⁶; Tim Van Den Bossche⁵; Andrew R Jones⁷; Pierre-Alain Binz⁸; Shin Kawano⁹; Luis Mendoza¹⁰; Nuno Bandeira¹¹; Jeremy Carver¹¹; Benjamin Pullman¹¹; Zhi Sun¹⁰; Nils Hoffmann¹²; Jim Shofstahl¹³; Yunping Zhu¹⁴; Helge Hecht¹⁵; Eric Deutsch¹⁰; Juan Antonio Vizcaino¹⁶; ¹Hong Kong University of Science and Technology, Hong Kong, Hong Kong; ²National Institute of Standards and Technology, Gaithersburg, MD; ³Boston University School of Medicine, Boston, MA; ⁴University of Antwerp, Antwerpen, Belgium; ⁵VIB-UGent Center for Medical Biotechnology, Gent, Belgium; ⁶European Molecular Biology Laboratory (EMBL), Heidelberg, Germany; ⁷University of Liverpool, Liverpool, United Kingdom; ⁸Lausanne University Hospital, Lausanne, Switzerland; ⁹Kitasato University, Kitasato, Japan; ¹⁰Institute for Systems Biology, Seattle, WA; ¹¹University of California San Diego, San Diego, CA; ¹²Forschungszentrum Jülich, Jülich, Germany; ¹³Thermo Fisher Scientific, San Jose, California; ¹⁴National Center for Protein Sciences (The PHOENIX Center, Beijing), Beijing, China; ¹⁵Masaryk University, Brno, Czech Republic; ¹⁶European Molecular Biology Laboratory, Heidelberg, Germany
- TP 391 **ADAP informatics for untargeted mass spectrometry-based metabolomics and exposomics big data**; Aleksandr Smirnov¹; Joel Hall¹; Toan Nguyen¹; Yunfei Liao²; Daisy Brumit¹; Yuanyuan Li³; Blake Rushing³; Susan McRitchie³; Radha Krishna Balaji¹; Komal Madamwar¹; Varun Suresh¹; Shanmukh Gorle²; Anantnaval Gaikwad¹; Steffy Roselina Eben Judson¹; Susan Sumner³; Xiuxia Du²; ¹University of North Carolina at Charlotte, Charlotte, North Carolina; ²University of North Carolina at Charlotte, Charlotte, NC; ³University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 392 **Automated and Scalable Cloud-Based Computational Pipeline for Large-scale Unbiased Plasma Proteomics Study**; Joon-Yong Lee¹; Jinlyung Choi¹; Sara Nouri Golmaei¹; Yuntao Hu¹; Sai Ramaswamy¹; Dijana Vitko¹; Wan-Fang Chou¹; Megan Mora¹; Jessica Chan¹; Mark Marispini¹; Benjamin Ta¹; Peter Spiro¹; Hoda Malekpour¹; Ajinkya Kokate¹; Robert Zawada¹; Bruce Wilcox¹; Philip Ma¹; Chinmay Belthangady¹; Manway Liu¹; ¹PrognomiQ Inc, San Mateo, CA
- TP 393 **A custom web-based bioinformatic tool for the assessment of potential molecular glues screened by quantitative discovery proteomics**; Daryl N Bulloch¹; Han-Yin Yang¹; Aman Makaju²; Ishwar N Kohale¹; Bradford Gibson¹; ¹Amgen, South San Francisco, CA; ²Amgen, Thousand Oaks, CA
- TP 394 **Evaluation of a Portable GC-MS for Drug Screening of Products Seized During a Simultaneous Nationwide Mail Blitz**; Lisa M. Lorenz¹; Michael D. Thatcher¹; Megan E. Sterling¹; ¹Food and Drug Administration, Office of Regulatory Affairs, Forensic Chemistry Center, Cincinnati, OH
- TP 395 **Portable MALDI-TOF Mass Spectrometer for Bioaerosol Detection**; Vadym Berkout¹; Stuart Collymore¹; Scott Ecelberger¹; Max Cetta¹; Lara Moore¹; Caroline Haddaway¹; Wayne Bryden¹; Mike McLaughlin¹; ¹Zeteo Tech, Inc., Sykesville, MD
- TP 396 **Technology Advancements for the Extraterrestrial Molecular Indicators of Life Investigation (EMILI) Capillary Electrophoresis Ionization Mass Spectrometer**; Desmond A. Kaplan^{1,2}; Maria Fernanda Mora³; Tomas Drevinskas³; Marco E. Castillo^{1,4}; Ryan M. Danell^{1,5}; Jacob D Graham¹; Friso Van Amerom^{1,6}; Xiang Li¹; Andrej Grubisic¹; Bethany P Theiling¹; Aaron C Noell⁷; Antonio J Ricco⁸; William B Brinckerhoff¹; Peter A Willis³; ¹National Aeronautics and Space Administration Goddard Space Flight Center, Greenbelt, MD; ²KapScience LLC, TEWKSBURY, MA; ³Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA; ⁴Aerodyne, Cape Canaveral, FL; ⁵Danell Consulting, Winterville, NC; ⁶Mini-Mass Consulting, Inc, Hyattsville, MD; ⁷National Aeronautics and Space Administration Jet Propulsion Laboratory, Pasadena, CA; ⁸National Aeronautics and Space Administration AMES, Mountain View, CA
- TP 397 **MOMA Testbed Instrument Characterization under Mars Conditions and Engineering Test Unit Sample Database Generation**; Friso H. W. Van Amerom^{1,2}; Xiang Li²; Marco E. Castillo^{2,3}; Ryan M. Danell^{2,4}; Desmond A. Kaplan^{2,5}; Andrej Grubisic²; William B. Brinckerhoff²; And The Moma Team⁶; ¹Mini-Mass Consulting, Inc, Hyattsville, MD; ²NASA Goddard Space Flight Center, Greenbelt, MD; ³ASES, Beltsville, MD; ⁴Danell Consulting, Winterville, NC; ⁵KapScience LLC, TEWKSBURY, MA; ⁶Max-Planck-Institut für Sonnensystemforschung, Göttingen, Germany

TUESDAY POSTERS

- TP 398 **Amino Acid Quantitation of Cell Culture Media Matrices via an Integrated CE-MS Analyzer**; Ji Young L Anderson¹; William Morgan-Evans²; Bethany Kerr²; Kenion H Blakeman¹; Milla Neffling¹; Graziella Piras¹; ¹908 Devices, Inc., Boston, MA; ²CPI Innovation Services Ltd., Darlington, United Kingdom
- TP 399 **Prototype Development of a Digital Linear Ion Trap based Portable GCMS for VOCs Analysis**; Chenzhang Zhu¹; Lin Liu¹; Hongbing Cheng¹; Yulei Hu¹; Xinfeng Zhou¹; Wenjian Sun¹; ¹Shimadzu Research Laboratory, Shanghai, China
- TP 400 **Interfacing and Characterizing Portable HPLC Interfaced with Miniature Ion Trap Mass Spectrometer**; Vladimir M Doroshenko¹; Victor Laiko¹; Venkateswara Panchagnula¹; Matthew Morse²; John Stimus²; ¹MassTech, Inc., Columbia, MD; ²Axcend LLC, Provo, UT
- TP 401 **Intelligent Miniature Mass Spectrometry System for Point-of-Care Analysis**; Bin Jiao¹; Yikun Liu¹; Xinwei Liu¹; Jiexun Bu²; Wenpng Zhang¹; Zheng Ouyang¹; ¹Tsinghua University, Beijing, China; ²PURSPEC Technology (Beijing) Ltd., Beijing, China
- TP 402 **Portable Mass Spectrometer for air born particle detection**; Chung-Hsuan Chen¹; Chun-Jen Hsiao Hsiao²; Ju-Yao Chang¹; Jung-Lee Lin²; Abdil Ozdemir³; ¹National Sun Yat-Sen University, Kaohsiung City, Taiwan; ²Academia Sinica, Taipei, Taiwan; ³Sakarya University, Sakarya, Turkey
- TP 403 **Modification of a Thermo LTQ-XL to Enable Automatic Gain Control and On-Demand 2D-MS/MS**; Eric T Dziekonski¹; R. Graham Cooks¹; ¹Purdue University, WEST LAFAYETTE, IN
- TP 404 **Theory and Performance of a Novel High-Resolution Mass Analyzer**; Hamish Stewart¹; Christian Hock¹; Dmitry Grinfeld¹; Matthias Biel¹; Philipp Cochems¹; Alexander Wagner¹; Wilko Balschun¹; Alexander Makarov¹; ¹Thermo Fisher Scientific, Bremen, Germany
- TP 405 **In Search of the Perfect Notch: a Novel Approach to the Optimization of Dipole Excitation Waveforms in Quadrupole Mass Filters**; Keith Richardson¹; Martin Green¹; David Langridge¹; ¹Waters Corporation, Wilmslow, United Kingdom
- TP 406 **Analysis of Megadalton ions using a novel dual sector Charge Detection Mass Spectrometer (CDMS)**; John B Hovyes¹; Dimitris Papanastasiou²; Alexandros Lekkas²; Yury Tsybin³; Anton Kozhinov³; Igor Filippov⁴; ¹TrueMass, Rowarth, United Kingdom; ²Fasmatech, NCSR Demokritos, Athens, Greece; ³Spectroswiss, Lausanne, Switzerland; ⁴MSCUBE Ltd, Auckland, New Zealand
- TP 407 **Mimicking the effects of pre-/post-filters by duty cycle manipulation on a single digitally operated mass filter**; Sumeet S Chakravorty¹; Elizabeth Groetsema¹; Fatima Olayemi Obe¹; Gordon Anderson²; Peter T. A. Reilly¹; ¹Washington State University, Pullman, WA; ²GAA Custom Electronics, LLC, Benton City, WA
- TP 408 **Developing the trap/filter/eject methodology for isolation and mass analysis in higher stability zones**; Elizabeth Groetsema¹; Sumeet Chakravorty¹; Fatima Olayemi Obe¹; Gordon Anderson²; Peter T. A. Reilly¹; ¹Washington State University, Pullman, WA; ²GAA Custom Electronics, LLC, Benton City, WA
- TP 409 **Genetic algorithm parallel optimization high-resolution planar electrostatic ion trap mass analyzer**; Weimin Wang¹; Fuxing Xu¹; Li Ding¹; Chuan-Fan Ding¹; ¹Ningbo University, Ningbo, China
- TP 410 **Integration of a SLIM-based High Resolution Ion Mobility Prototype with an Orbitrap Mass Spectrometer**; Alan A McKenzie-Coe¹; Liulin Deng²; Brian Adamson³; Kyle L. Fort⁴; Eloy R Wouters³; Gordon A Anderson⁵; Lee Earley⁶; Jean-Jacques Dunyach⁷; Daniel Debord²; Alexander A Makarov⁴; ¹MOBILion Systems, Inc., Chadds Ford, PA; ²MOBILion Systems, Inc, Chadds Ford, PA; ³Thermo Fisher Scientific, San Jose, California; ⁴Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ⁵GAA Custom Electronics, LLC, Benton City, WA; ⁶Thermo Fisher Scientific, Boston, MA; ⁷ThermoFisher Scientific, San Jose, CA
- TP 411 **Configuration and Deployment of The Shimadzu TQ8040 Triple Quad as an Atmospheric Monitoring Real-Time High-Definition Mass Spectrometer (3Q-RTHD-MS)**; Karl K Weitz¹; Bryson Gibbons¹; Rosalie K. Chu¹; James J Moran^{1,2}; Ljiljana Pasa-Tolic¹; Amirhossein H. Ahkami¹; Kirsten S. Hofmocker¹; Janet K. Janssen¹; Mary S Lipton¹; ¹Battelle Pacific Northwest National Laboratories, Richland, WA; ²Michigan State University, East Lansing, MI
- TP 412 **A Novel Digital Waveform Generator for Creating High Resolution, Low Jitter, Rectangular Waveforms**; Gordon Anderson¹; Sumeet Chakravorty²; Fatima Obe²; Elizabeth Groetsema²; Peter T. A. Reilly²; ¹GAA Custom Electronics, LLC, Benton City, WA; ²Washington State University, Pullman, WA
- TP 413 **Conquering Waveform-to-Waveform Reproducibility to Improve Digital Waveform Mass Analysis at High Mass in Higher Stability Zones**; Peter T. A. Reilly¹; Sumeet S Chakravorty¹; Fatima Olayemi Obe¹; Elizabeth Groetsema¹; Gordon Anderson²; ¹Washington State University, Pullman, WA; ²GAA Custom Electronics, LLC, Benton City, WA
- TP 414 **Using a branched RF-ion trap to combine EAD, ultraviolet-photodissociation (UVPD) and CID fragmentation**; Mircea Guna¹; Pavel Ryumin¹; Anjali Chelur¹; Nick Albeanu¹; Takashi Baba¹; Yves Le Blanc²; ¹SCIEX, Concord, ON; ²SCIEX, Concord, ON, ON
- TP 415 **Improving the Efficiency of Isolation of Native Protein Complexes by a Digital Mass Filter**; Robert Schrader¹; David Russell¹; ¹Texas A&M University, College Station, TX
- TP 416 **Process monitoring and control using a Time-of-Flight Mass spectrometer in both electron ionization and ion energy spectrometer configurations**; Abdelhak Bensaoula¹; Patrick Sturm¹; Janos Metzger¹; Carsten Stoemer¹; Chia-Yu Tzou¹; Georgios Papadopoulos¹; Caroline Hain²; Thomas Nelis²; Jonathan Thomet³; ¹Tofwerk AG, Thun, Switzerland; ²Berner Fachhochschule BFH, Biel, Switzerland; ³Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland
- TP 417 **Application of the Digital Tandem Mass Filter in Native Spray Analysis of Proteins**; Fatima Olayemi Obe¹; Sumeet S. Chakravorty¹; Elizabeth Groetsema¹; Gordon A. Anderson²; Peter T. A. Reilly¹; ¹Washington State University, Pullman, WA; ²GAA Custom Electronics, LLC, Benton City, WA
- TP 418 **Real-Time Optimization of Ultra-High Resolution in Charge Detection Mass Spectrometry**; David Reitenbach¹; Daniel Y Botamanenko²; Martin F. Jarrold²; ¹Indiana University, Bloomington, IN; ²Indiana University Bloomington, Bloomington, IN
- TP 419 **Impact of high temperature ion source gas: thermal protein denaturation and finer structural details at lower collisional induced unfolding energies**; Mack Shih¹; Patrick J Faustino¹; Thomas O'Connor¹; Xiaoming Xu¹; Jinhui Zhang¹; ¹Food and Drug Administration, Silver Spring, MD
- TP 420 **Trapped Ion Mobility Spectrometry (tims) Facilitates Lipid and Metabolite Identification in MALDI Mass Spectrometry Imaging**; Min Liu¹; Carolina Cruz Cepeda¹; John M Koomen¹; ¹Moffitt Cancer Center, Tampa, FL
- TP 421 **Developing tandem mass spectrometry file structures for ion mobility spectrometry workflows**; Bryson Gibbons¹; Sarah Stow²; Ruwan T Kurulugama²; Lauren Royer³; Daniel Debord³; John C Fjeldsted²; Richard D. Smith¹; Aivett Bilbao¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²Agilent Technologies, Santa Clara, CA; ³MOBILion Systems, Inc., Chadds Ford, PA
- TP 422 **Implementation of a Highly Modular Structures for Lossless Ion Manipulations-Time-of-Flight Mass**

TUESDAY POSTERS

- Spectrometry Platform; Zackary R Kinlein¹; Cullen Greer¹; Brian H. Clowers¹; ¹Washington State University, Pullman, WA**
- TP 423 **Development of Top Down Protein Analysis using Trapped Ion Mobility with Two-Dimensional Mass Spectrometry with UVPD and IRMPD; Callan Littlejohn¹; Meng Li²; Christopher A. Wootton^{2,3}; Peter B. O'Connor²; ¹University of Warwick, Coventry, United Kingdom; ²University of Warwick, Coventry, United Kingdom; ³Bruker Daltonics, Bremen, Germany**
- TP 424 **Differentiation and Visualization of Chiral Amino Acids Using Ion Mobility Mass Spectrometry; Chengyi Xie^{1,2}; Yanyan Chen^{1,2}; Xiaoxiao Wang^{1,2}; Yuting Shen^{1,2}; Yuanyuan Song^{1,2}; Xin Diao^{1,2}; Lin Zhu^{1,2}; Jianing Wang^{1,2}; Zongwei Cai^{1,2}; ¹State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, China; ²Department of Chemistry, Hong Kong Baptist University, Hong Kong, China**
- TP 425 **Reproducibility of drift gas modifier effects in atmospheric pressure drift tube ion mobility spectrometry of small molecules; Matthew Carlo¹; Amanda Patrick¹; ¹Mississippi State University, Mississippi State, MS**
- TP 426 **A Dual-Gated Structures for Lossless Ion Manipulations Ion Mobility Orbitrap Mass Spectrometry Platform for Simultaneously Acquiring High-Resolution IM-MS-HCD Data Sets; Adam L. Hollerbach¹; Yehia M. Ibrahim¹; Vanessa M. Meras¹; Randolph V. Norheim¹; Adam P. Huntley¹; Gordon Anderson²; Thomas O. Metz¹; Robert G. Ewing¹; Richard D. Smith¹; ¹Pacific Northwest National Laboratory, Richland, WA; ²GAA Custom Electronics, LLC, Benton City, WA**
- TP 427 **An interplatform study of three ion mobility techniques to determine lipid collision cross sections; Anaïs C. George¹; Isabelle Schmitz²; Vincent Marie²; Benoît Colsch²; Florent Rouvière³; Sandra Alves⁴; Sabine Heinisch³; François Fenaille²; Carlos Afonso¹; Corinne Loutelier-Bourhis¹; ¹Laboratoire COBRA, UMR 6014, Université de Rouen, INSA de Rouen, CNRS, IRCOF, Mont Saint Aignan, France; ²Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), MetaboHUB, F-91191 Gif sur Yvette, France; ³Université de Lyon, Institut des Sciences Analytiques, UMR 5280 CNRS, 5 rue de la Doua, 69100 Villeurbanne, France; ⁴Sorbonne Université, Faculté des Sciences et de l'Ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France**
- TP 428 **A Comprehensive TWIM Calibration Method for Obtaining High-Throughput Multi-Omic Collision Cross Section Values; Hannah M Hynds¹; Jana M Carpenter¹; Kelly M Hines¹; ¹University of Georgia, Athens, GA**
- TP 429 **Development of a high-resolution U-shaped mobility analyzer (UMA) and its applications; Xiaogiang Zhang¹; Kuofeng Tseng¹; Kang Guo¹; Yangyue Miao¹; Lin Liu¹; Xinfeng Zhou¹; Wenjian Sun¹; ¹Shimadzu Research Laboratory, Shanghai, China**
- TP 430 **TW-SLIM Separations Using Asymmetric Radio-Frequency Trapping Fields; Cullen Greer¹; Zackary R. Kinlein¹; Brian H. Clowers¹; ¹Washington State University, Pullman, WA**
- TP 431 **Novel concept of sliding ion mobility windows to increase the resolution in trapped ion mobility-mass spectrometry hyphenated with gas chromatography; Hugo Muller¹; Georges Scholl¹; Johann Far¹; Edwin De Pauw¹; Gauthier Eppe¹; ¹University of Liège, Liège, Belgium**
- TP 432 **Experimental and theoretical determination of the collision cross sections of phosphoric acid clusters: anions compared to cations; Héléne Lavanant¹; Valentina Calabrese²; Frédéric Rosu³; Valérie Gabelica⁴; Carlos Afonso¹; ¹Normandie Univ, UNIROUEN, INSA Rouen, CNRS, COBRA, Rouen, France; ²University of Lyon, University Claude Bernard 1 of Lyon, Institute of Analytical Sciences, CNRS UMR 5280, Villeurbanne, France; ³CNRS, UMS 3033, Institut Européen de Chimie et Biologie (IECB), Pessac, France; ⁴University of Bordeaux, INSERM and CNRS, ARNA Laboratory, IECB site, Pessac, France**
- TP 433 **Millions and Millions of Ions: An Improved Guard Design and Giant Ion Trap to Enhance SLIM Sensitivity and Duty Cycle; Joshua K McBee¹; Liulin Deng¹; Adam Engelson¹; Zongyuan Chen¹; Daniel Deboard¹; ¹MOBILion Systems, Inc, Chadds Ford, PA**
- TP 434 **Nonlinear Fourier Transform Sweeps in Conjunction with Reduced-Pressure Ion Mobility Mass Spectrometry; Nathan W. Buzitis¹; Elvin R. Cabrera¹; Brian H. Clowers¹; ¹Washington State University, Pullman, WA**
- TP 435 **Real-time monitoring of dynamic isomer populations with CI-SLIM IMS-MS; Sonja Klee¹; Felipe Lopez-Hilfiker¹; Matthieu Riva^{1,2}; Sebastian Gerber¹; Urs Rohner¹; Stephan Graf¹; Michael Z. Kamrath¹; ¹TOFWERK, Thun, Switzerland; ²Univ. Lyon, Université Claude Bernard Lyon 1, Villeurbanne, France**
- TP 436 **Large-scale inference of Peptide Collisional Cross-Sections in an Orbitrap mass analyzer; Ulises Hernandez Guzman¹; Konstantin Ayzikov²; Kyle L. Fort²; Martin Rykaer¹; Jeppe Madsen¹; Ana Martinez Del Val¹; Alexander A Makarov²; Jesper V. Olsen¹; ¹Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany**
- TP 437 **Low-Cost, Open-Source Multiplexing Platform for Ion Gate Control on High Kinetic Energy Ion Mobility Spectrometry (HiKE-IMS) to Increase Ion Throughput; Cameron N Naylor¹; Brian H. Clowers²; Florian Schlottmann¹; Nic Solle¹; Stefan Zimmermann¹; ¹Leibniz Universität Hannover, Institut für Grundlagen der Elektrotechnik und Messtechnik, Hannover, Germany; ²Washington State University Department of Chemistry, Pullman, WA**
- TP 438 **A new TIMS-MRMS instrument for structural and in-situ analysis of biomolecules; Anna L Simmonds¹; Anthony Devlin²; Alina Theisen³; Gregory Brabeck³; Carlos Schat³; Christopher A. Wootton³; Josephine Bunch^{2,4}; Zoltan Takats^{2,5}; ¹Rosalind Franklin Institute, Didcot, United Kingdom; ²Rosalind Franklin Institute, Harwell, Didcot, United Kingdom; ³Bruker Daltonics GmbH & Co.KG, Bremen, Germany; ⁴National Physical Laboratory, Teddington, United Kingdom; ⁵Imperial College London, London, United Kingdom**
- TP 439 **CIUSuite 3: Next-generation CCS Calibration and Automated Data Analysis tool for Gas-phase Protein Unfolding; Chae Kyung Jeon¹; Carolina Rojas Ramirez¹; Ruwan T Kurulugama²; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, MI; ²Agilent Technologies, Santa Clara, CA**
- TP 440 **Exploring the structures and the energy landscapes of proteins in the gas phase through chemical modification and ion mobility; Thomas Tilmant¹; Johann Far¹; Edwin De Pauw¹; Loic Quinton¹; ¹MSLab ULiège, Liège, Belgium**
- TP 441 **20 mM Ammonium Carbonate Improves the Detection of Tricarboxylic Acid Cycle Intermediates; Jarrod A Roach¹; Laura-Isobel McCall²; ¹University of Oklahoma, Norman, OK; ²University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK**
- TP 442 **Online 2D high-pH and low-pH reversed-phase nano-LC-MS/MS system for deep proteome analysis; Chao-Jung Chen¹; Yu-Ching Liu¹; ¹China Medical University, Taichung, Taiwan**
- TP 443 **RP-LC gradient method development and gradient elution modelling to optimize complex mixture analysis by high-resolution mass spectrometry; Leila Afjehi¹; Steffen Waldherr²; ¹University of Vienna/Mass Spectrometry Core Facility- CF SS, Vienna, Austria; ²University of Vienna/**

TUESDAY POSTERS

- Department of Functional and Evolutionary Ecology, Vienna, Austria
- TP 444 **ISDL.CSA: MS1 Composite Spectra Analysis to Complement MS2 Annotation in Untargeted Metabolomics Datasets;** Sadjad Fakouri Baygi¹; Yashwant Kumar²; Dinesh Kumar Barupal¹; ¹*Icahn School of Medicine at Mt Sinai, New York, New York, United States, NY*; ²*Non-communicable Diseases Division, Translational Health Science and Technology Institute, Faridabad, Haryana, India*
- TP 445 **High-throughput analysis with improved proteome coverage using new designed micro pillar array column (µPAC);** Xuefei Sun¹; Yuan Lin¹; Jeff Op De Beeck²; Brandon H. Robson¹; Joshua A Silveira³; Paul Jacobs²; Shanhua Lin¹; ¹*Thermo Fisher Scientific, Sunnyvale, CA*; ²*Thermo Fisher Scientific, Ghent, Belgium*; ³*Thermo Fisher Scientific, San Jose, CA*
- TP 446 **Increasing Efficiency of Peptide Separations by Decreasing Particle Size and Column Dimension;** Peter Pellegrinelli¹; Benjamin Libert¹; Stephanie Schuster¹; Conner McHale¹; ¹*Advanced Materials Technology, Wilmington, DE*
- TP 447 **Coupling normal phase chromatographic separation with electron ionization in low and high-resolution mass spectrometry via liquid electron ionization interface;** Genny Grasselli¹; Adriana Arigo¹; Nicole Marittimo¹; Giorgio Famigliini¹; Pierangela Palma^{1,2}; Mansoor Saeed³; Simon Perry³; Pablo Navarro³; Phil Clarke³; Mark Brittin³; Achille Cappiello^{1,2}; ¹*UNIVERSITY OF URBINO CARLO BO, URBINO, Italy*; ²*Vancouver Island University, Nanaimo, BC*; ³*Syngenta Jealott's Hill International Research Centre, Bracknell, United Kingdom*
- TP 449 **Improved Biopolymer LCMS Using a New Mixed-Mode Chromatographic Stationary Phase;** Benjamin Libert¹; Barry E Boyes¹; Chuping Luo¹; Marc Goldfinger¹; Mark Haynes¹; ¹*Advanced Materials Technology, Wilmington, DE*
- TP 450 **Robust profiling of crude and undepleted human plasma using µPAC-based high resolution DIA-MS workflow;** Jeff Op De Beeck¹; Natalie Van Landuyt¹; Delphi Van Haver^{2,3}; An Staes^{2,3}; Francis Impens^{2,3}; Xuefei Sun⁴; Yuan Lin⁴; Paul Jacobs¹; ¹*Thermo Fisher Scientific, Zwijnaarde, Belgium*; ²*VIB Proteomics Core, Ghent, Belgium*; ³*Department of Biomolecular Medicine, Ghent University, Ghent, Belgium*; ⁴*Thermo Fisher Scientific, Sunnyvale, CA*
- TP 451 **The Development of a Virtual Liquid Chromatography Method Development Tool;** Melinda D Ulrich¹; Jamie York¹; John Garrett¹; Chris Nelson¹; Justin Steimling¹; Tim Yosca¹; ¹*Restek Corporation, Bellefonte, PA*; ²*Analytical Innovations, Inc., Dayton, OH*
- TP 452 **Optimizing LCMS Method Development for Oligonucleotide Separations: Advantages of Bio Compatible UHPLC Systems;** Patrick Cronan; *Agilent, Lexington, MA*
- TP 453 **Simultaneous determination of 85 fentanyl analogues using liquid chromatography-tandem mass spectrometry (LC-MS/MS) with serially coupled columns;** Jiyu Kim¹; Sang Beom Han¹; ¹*Dept of Pharmaceutical Analysis, College of Pharmacy, Chung-Ang University, Seoul, South Korea*
- TP 454 **Very Weak Anion Exchange (VWAX) Chromatography for Glycopeptide Enrichment and Separation;** Danqing Wang¹; Peng-Kai Liu²; Ting-Jia Gu³; Bin Wang³; Andrew J. Alpert⁴; Lingjun Li^{1,2,3}; ¹*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*; ²*Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI*; ³*School of Pharmacy, University of Wisconsin-Madison, Madison, WI*; ⁴*PolyLC Inc., Columbia, MD*
- TP 455 **Hydrophilic Interaction Chromatography for Improved LC-MS/MS Analysis of Intact Protamines;** Melissa R. Leyden¹; Donald F. Hunt^{1,2}; Jeffrey Shabanowitz¹; ¹*Department of Chemistry, University of Virginia, Charlottesville, VA*; ²*Department of Pathology, University of Virginia, Charlottesville, VA*
- TP 456 **Sample dilution in microLC sample loops: solving solvent/matrix peak shape artifacts during high-load liquid microchromatography/triple-quadrupole mass spectrometry of Fmoc-amino acids;** John J Thaden; *Texas A&M University - Center for Translational Research in Aging and Longevity, College Station, TX*
- TP 457 **Filtering utility for grouping untargeted mass spectrometry datasets (FUGU-MS): an open-source software tool for metabolomics;** Raied Aburashed¹; Thomas Rydzak¹; Saad Luqman¹; Ian A Lewis¹; ¹*University of Calgary, Calgary, AB*
- TP 458 **Intelligent Reflex Fast Screening for Drugs in Urine: data-dependent reinjection logic for screening and confirmation of presumptive positives;** Patrick Batoon¹; Lee Bertram²; Linfeng Wu²; ¹*Agilent Technologies Inc., Santa Clara, CA*; ²*Agilent Technologies, Santa Clara, CA*
- TP 459 **FidelityCheck™ Software: Reversed-Phase Retention Time Modeling for Modified and Variant Peptide Identification;** Tyler Fletcher¹; Jiana Duan¹; Emily Chea¹; Robert Egan¹; Ron Orlando^{1,2}; Scot Weinberger¹; ¹*GenNext Technologies, Half Moon Bay, CA*; ²*University of Georgia, Athens, GA*
- TP 460 **Tackling Cannabinoids Ion Suppression Issues in Biological Matrices Using Chromatographic Tools;** Cynthia Côté¹; Stephanie Savard¹; Cynthia Dombrowski¹; Eugénie-Raphaëlle Bérubé¹; Gabrielle Daigneault¹; Pierre-Yves Martin¹; Julie Laquerre¹; Pascal Mireault¹; ¹*Laboratoire de sciences judiciaires et de médecine légale, Montreal, QC*
- TP 461 **Retention Time Prediction for O-GlcNAc Serine and Threonine Carrying Peptides;** Quinn K Neale¹; Darien Yeung¹; Victor Spicer¹; Helene Perreault¹; Oleg V. Krokhin¹; ¹*University of Manitoba, Winnipeg, MB*
- TP 462 **Rapid fractionation of human proteome with acidic HILIC Proteome Selective Isolation Chromatography (P-SLIC) by TMT-based quantitation;** Darien Yeung^{1,2}; Ying Lao^{1,2}; Victor Spicer^{1,2}; Oleg V. Krokhin^{1,2}; ¹*Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB*; ²*University of Manitoba, Winnipeg, MB*
- TP 463 **To study the in-vitro and in-vivo effects of Bergamottin and Diosmetin on amoxapine metabolism using LC-MS/MS and LCHR-MS/MS;** Sachin Dattam Paware¹; Dr.pramod Kumar¹; ¹*National Institute of Pharmaceutical Education and Research Guwahati (NIPER-G), Guwahati, India*
- TP 464 **Fast and Targeted Analysis of Cell Culture Media Components using QSight LC/MS/MS;** Marc R Elie¹; Cole Stratman¹; Jacob Jalali¹; Jesse Leonard²; Erasmus Cudjoe³; ¹*Perkin Elmer, Shelton, CT*; ²*PerkinElmer, Shelton, CT*; ³*PerkinElmer Inc., Woodbridge, ON*
- TP 465 **The investigation of tryptophan metabolites and vitamin B in human and murine tissue via high-resolution mass spectrometry;** Sandy Abujrais¹; Kumari Ubhayasekeraa¹; Jonas Bergquist¹; ¹*Uppsala University, uppsala, Sweden*
- TP 466 **Analysis of short-chain fatty acids (SCFAs) by LC-MS/MS coupled with chemical derivatization;** Hanpeng Jiang¹; Zhimin Long¹; Lihai Guo¹; ¹*SCIEX, China, Shanghai, China*
- TP 467 **Rapid analysis of 11 energy-rich phosphate compounds using the SCIEX Triple Quad 6500+ system;** Junmiao Chen¹; Dandan Si¹; Zhimin Long¹; ¹*SCIEX, Beijing, China*
- TP 468 **Simultaneous analysis of polar metabolome and lipidome by unified-hydrophilic interaction/anion-exchange liquid chromatography tandem mass spectrometry (unified-HILIC/AEX/MS/MS);** Kohta Nakatani¹; Kazuki Ikeda¹; Masatomo Takahashi¹; Takeshi Bamba¹; Yoshihiro Izumi¹; ¹*Medical Institute of Bioregulation, Fukuoka, Japan*

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- TP 469 **Targeted analysis of energy metabolites in cells using liquid chromatography-tandem mass spectrometry;** Xiaoyuan Shi¹; Zhimin Long¹; Lihai Guo²; ¹SCIEX, China, Shanghai, China; ²SCIEX, China, Beijing, China
- TP 470 **Determination of Flux into the Tryptophan-Kynurenine Pathway in Biological Samples using Liquid Chromatography Tandem Mass Spectrometry;** Jaeman Byun¹; Subramaniam Pennathur¹; Anna Mathew¹; ¹University of Michigan, Ann Arbor, MI
- TP 471 **Chiral chromatography in conjunction with LC-MRM-MS for enantiomer-specific resolution of the oxylipidome;** Liping Yang¹; Jaewoo Choi²; Jan F. Stevens³; Claudia Maier^{1,2}; ¹Department of Chemistry, Oregon State University, Corvallis, OR; ²Linus Pauling Institute, Oregon State University, Corvallis, OR; ³Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR
- TP 472 **Multiple Reaction Monitoring (MRM) Method Development for Quantitation of Spermidine in Whole Blood;** Jericha Mill¹; Cameron Kaminsky¹; Thomas Raife²; Lingjun Li^{1,3}; ¹University of Wisconsin-Madison, Department of Chemistry, Madison, WI; ²University of Wisconsin School of Medicine and Public Health, Department of Pathology and Laboratory Medicine, Madison, WI; ³University of Wisconsin-Madison, School of Pharmacy, Madison, WI
- TP 473 **Measurement of Phthalates using Liquid Chromatography-Mass Spectrometry;** Abu Hena Mostafa Kamal¹; Vasanta Putluri²; Chandra Shekar Reddy Ambati²; Bhagavatula Moorthy²; Chris Amos²; Nagireddy Putluri²; ¹Baylor College of Medicine, Houston, TX; ²Baylor College of Medicine, Houston, Texas
- TP 474 **Wide-Target Analysis of Yogurt Using Triple Quadrupole LC-MS/MS;** Yuki Ito^{1,2}; Jun Watanabe^{1,2}; Junko Iida^{1,2}; ¹SHIMADZU Corporation, Kyoto, Japan; ²Osaka University Shimadzu Omics Innovation Research Laboratories, Suita, Japan
- TP 475 **High-throughput UHPLC-MS/MSMRM amino acid and acylcarnitine profiling in early infancy predicts later obesity risk;** Susanne I. Wudy¹; Verena K. Mittermeier-Kleßinger¹; Sapna Sharma¹; Andreas Dunkel²; Karin Kleigrew³; Regina Ensenaue^{4,5,6}; Corinna Dawid^{1,3}; Thomas F. Hofmann¹; ¹Chair of Food Chemistry and Molecular Sensory Science, Technical University of Munich, Freising, Germany; ²Leibniz-Institute for Food Systems Biology at the Technical University of Munich, Freising, Germany; ³Bavarian Center for Biomolecular Mass Spectrometry, Technical University of Munich, Freising, Germany; ⁴Institute for Medical Information Processing, Biometry, and Epidemiology (IBE), Ludwig-Maximilians-Universität München, Munich, Germany; ⁵Division of Pediatric Cardiology and Intensive Care, University Hospital, Ludwig-Maximilians-Universität München, Munich, Germany; ⁶Institute of Child Nutrition, Max Rubner-Institut, Federal Research Institute of Nutrition and Food, Karlsruhe, Karlsruhe, Germany
- TP 476 **Development and Optimization of Lipidomic Studies Utilizing the SICRIT® LC-Module;** Ciara Conway¹; Jan-Christoph Wolf²; Christoph Haisch³; ¹UNC Charlotte, CHARLOTTE, NC; ²Plasmion GmbH, Augsburg, Germany; ³Technical University of Munich, Freising, Germany
- TP 477 **Analysis of biological samples by fast HILIC separations of nucleotides, and RPLC separation of 3-NPH derivatized carboxylic acids with LC-MS/MS;** Ondrej Hodek^{1,2}; Thomas Moritz³; ¹Department of Forest Genetics and Plant Physiology, Swedish University of Agricultural Sciences, Umeå, Sweden; ²Swedish Metabolomics Centre, Umeå, Sweden; ³Novo Nordisk Foundation Center for Basic Metabolic Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark
- TP 478 **High Resolution LC-MS Method for Detecting and Quantifying Sterols and Sterol Adducts in Plant matrices;** Suresh Annangudi¹; Scott Greenwalt¹; Jeffrey Simpson¹; ¹Corteva Agriscience, Indianapolis, IN
- TP 479 **Reliable quantification of adenylyate nucleotides using ultra-performance liquid chromatography-tandem mass spectrometry (UPLC-MS/MS);** Maleesha De Silva¹; Kyle Fulghum¹; David Hoetker¹; Bradford G Hill¹; Pawel K Lorkiewicz¹; ¹University of Louisville, Louisville, KY
- TP 480 **Using targeted LC-MS/MS-based metabolomics to measure a broad spectrum of bile acids in disorders of human intestinal health;** Anthony Haag^{1,2}; Thomas D Horvath^{1,2}; Sigmund J Haidacher^{1,2}; Kathleen M. Hoch^{1,2}; Melinda A. Engevik³; Amy Engevik³; ¹Baylor College of Medicine, Houston, Texas; ²Texas Children's Hospital, Dept. of Pathology, Houston, Texas; ³Medical University of South Carolina, Charleston, SC
- TP 481 **Analysis of Polyamine Metabolism by Liquid Chromatography-High Resolution Mass Spectrometry;** Bao Tran¹; Lin Tan²; Thomas D Horvath³; Sara A Martinez¹; John Weinstein¹; Philip Lorenzi¹; ¹University of Texas MD Anderson Cancer Center, Houston, TX; ²MD Anderson Cancer Center, Houston, TX; ³Baylor College of Medicine, Houston, Texas
- TP 482 **Targeted metabolite analysis of polyamine synthesis and metabolism by LC-MRM/MS;** Katelyn G. McMurray¹; Jun Han^{1,2}; Juncong Yang¹; Molly McCormack¹; Gillian Leach¹; Kiara Kumar¹; Dave Schibli^{1,2}; David R. Goodlett^{1,3}; ¹Genome BC Proteomics Centre, University of Victoria, Victoria, BC; ²Division of Medical Sciences, University of Victoria, Victoria, BC; ³Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC
- TP 483 **Targeted quantitation of 400 polar metabolites of primary metabolism and energy homeostasis by LC-MRM/MS;** Jun Han^{1,2}; Juncong Yang¹; Molly McCormack¹; Kiara Kumar¹; Katelyn G. McMurray¹; Gillian Leach¹; Dave Schibli^{1,2}; David R. Goodlett^{1,3}; ¹Genome BC Proteomics Centre, University of Victoria, Victoria, BC; ²Division of Medical Sciences, University of Victoria, Victoria, BC; ³Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC
- TP 484 **A High-Efficiency Method for simultaneous Quantification of Seven Classes of Phytohormones;** Lingyun Chen¹; Yun Zhao¹; Qidan Li¹; Jin Zi¹; ¹BGI-Shenzhen, Shenzhen, China
- TP 485 **Targeted metabolic analysis of bile acids in biological samples by ultra-performance liquid chromatography tandem mass spectrometry;** Yun Zhao¹; Yang Feng¹; Hongkai Xu¹; Qidan Li¹; Jin Zi¹; ¹BGI-Shenzhen, Shenzhen, China
- TP 486 **LOD and LOQ determination of metabolites by using OT2 liquid handler and HILIC/PFP columns on a OrbitrapTMID-XTMMass Spectrometer;** Didar Asik¹; Vyncent Nguyen¹; Sarah Baron¹; Chengjian Tu¹; ¹Thermo Fisher Scientific, Grand Island, NY
- TP 487 **Comparison between pentafluorophenylpropyl and HILIC UHPLC-MS performance in cell culture media metabolite monitoring for untargeted metabolomic application;** Vyncent Nguyen¹; Chengjian Tu¹; ¹Thermo Fisher Scientific, Buffalo, NY
- TP 488 **Homogenization procedure optimizations for GI tract tissues collected from non-human primates for targeted metabolomics-based bioanalysis;** Sigmund J Haidacher^{1,2}; Erin E. Bolte³; Thomas D Horvath^{1,2}; Maxim Daniel Seferovic³; Kathleen M. Hoch^{1,2}; Derek Steven O'Neil³; James Versalovic^{1,2}; Anthony Haag^{1,2}; Kjersti Aagaard³; ¹Texas Children's Hospital - Microbiome Center, Houston, TX; ²Baylor College of Medicine, Houston, Texas; ³Department of Obstetrics & Gynecology, Division of Maternal-Fetal Medicine, Baylor College of Medicine, Houston, Texas
- TP 489 **Determination of ATP, ADP, AMP, and Adenosine Levels by Microchip Capillary Electrophoresis Coupled with High Resolution Mass Spectrometry;** Kevin Kun

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- TP 490 **Comparing Targeted LC-MS/MS and Untargeted GC-MS for the analysis of Kynurenine Pathway in Plasma Samples**; Luis M Valdiviez¹; Uri Keshet¹; Oliver Fiehn¹; ¹West Coast Metabolomics Center, Davis, CA
- TP 491 **Quantitative analysis of antimicrobial compounds from *Pseudomonas protegens***; Samantha J Balboa¹; Shilu Dahal²; Clemencia M. Rojas²; Leslie M. Hicks¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC; ²University of Nebraska-Lincoln, Lincoln, NE
- TP 492 **Quantitative Analysis of Polar Metabolites with Comprehensive Plasma and Cell Targeted Metabolomics Workflow**; Karen E Yannell¹; Cate Simmermaker¹; Genevieve C Van de Bittner¹; ¹Agilent Technologies, Santa Clara, CA
- TP 493 **Absolute quantitation of metabolites using machine learning and “standard candles” as universal calibrators - the second generation model**; Jennifer M Campbell¹; Timothy Kassis¹; Sofia Costa¹; Jeff Pruyne¹; Luke Ferro¹; Joshua D Lauterbach¹; Steven Hooper¹; Jack Howland¹; Gabriel Asher¹; Mimoun Cadosch Delmar¹; J. M. Geremia¹; ¹Matterworks, Somerville, MA
- TP 494 **Tracking metabolism in real time: an LC-MS enabled workflow that allows seconds-level resolution of metabolic fluxes in cell culture**; Ryan A Groves¹; Thomas Rydzak¹; Raied Aburashed¹; Stephanie L Bishop¹; Maryam Mapar¹; Carly C Y Chan¹; Ian A Lewis¹; ¹University of Calgary, Calgary, AB
- TP 495 **Absolute quantification of cellular metabolites in bioprocessing samples using machine learning**; Luke S Ferro¹; Jack Howland¹; Timothy Kassis¹; Ana S.H. Costa¹; Jeff Pruyne¹; Steven Hooper¹; Joshua D Lauterbach¹; Gabriel Asher¹; Mimoun Cadosch Delmar¹; J. M. Geremia¹; Jennifer M Campbell¹; ¹Matterworks, Somerville, MA
- TP 496 **High-Throughput Scheduled Parallel Reaction Monitoring Mass Spectrometry of Tryptophan-Indole Metabolites in Culture Supernatant of Human Bacterial Isolates**; Huidi Tian¹; Elizabeth Fleming²; Lina Kozhaya²; Rachel Hardy²; Derya Unutmaz²; Julia Oh²; Xudong Yao¹; ¹University of Connecticut, Storrs, CT; ²The Jackson Laboratory, Farmington, CT
- TP 497 **Delineating the natural product composition of Ashwagandha extracts by combining electrophile trapping with untargeted chemical fingerprinting and GNPS networking**; Md. Nure Alam¹; Armando Alcazar Magana¹; Jaewoo Choi¹; Luke Marney¹; Paul Cheong¹; Mikah Brandes²; Cody Neff²; Amala Soumyanath²; Jan F. Stevens¹; Claudia Maier¹; ¹Oregon State University, Corvallis, OR; ²Oregon Health & Science University, Portland, Oregon
- TP 498 **Analysis for Erinacines and Hericenones in Lion's Mane Mushrooms using HRMS and Ion Mobility**; Gordon T. Fujimoto¹; Sarah E. Dowd¹; Lindsay E. Hatch¹; Emily R. Britton¹; ¹Waters Corporation, Milford, Milford, MA
- TP 499 **Traditional and Vacuum Ionization MS for Characterization of Haustorium, Endosperm, Roots, Shoots and Leaves of Six-month old Germinating Coconut Seed**; Ellen D. Inutan¹; Kathleen C. Aligaya¹; Asia Catherine M. Mahayag¹; Johayber Sarip¹; Enjelyn C. Gomez¹; Sarah Trimpin²; Charles N. McEwen³; ¹Mindanao State University-Iligan Institute of Technology, Iligan City, Philippines; ²Wayne State University, Detroit, MI; ³Research and Development, MSTM, LLC, Philadelphia, Pennsylvania
- TP 500 **The Liquid Microjunction Surface Sampling Probe (LMJSSP) for Untargeted Secondary Metabolite Identification in Canadian Filamentous Soil Fungi**; Jessie Deng¹; Jennifer L Kolwich¹; Haidy Metwally¹; Avena C Ross¹; Richard D Oleschuk¹; ¹Queen's University, Kingston, ON
- TP 501 **Characterization of *Conus* textile crude venom by capillary electrophoresis hyphenated to mass spectrometry**; Fabrice Saintmont¹; Yoann Ladner¹; Sébastien Dutertre¹; Claudia Bich¹; ¹Univ. Montpellier, CNRS, ENSCM, IBMM, UMR5247, Montpellier, France
- TP 502 **Nontargeted UHPLC-TIMS-ToF-MS Analyses of American Elderberry (*Sambucus canadensis*) Fruits for Expanded Identification and Cultivar Comparisons**; Clayton Kranawetter^{1,2,3,4}; Barbara Sumner^{2,4}; Andrew L. Thomas⁵; Lloyd W. Sumner^{1,2,3,4}; ¹Department of Biochemistry, University of Missouri-Columbia, Columbia, MO; ²Metabolomics Center, University of Missouri-Columbia, Columbia, MO; ³Interdisciplinary Plant Group, University of Missouri-Columbia, Columbia, MO; ⁴Christopher S. Bond Life Sciences Center, University of Missouri-Columbia, Columbia, MO; ⁵Southwest Research Center, Division of Plant Sciences, University of Missouri, Columbia, MO
- TP 503 **Determination of polyphenols in American elderberry using HPLC-MS/MS, and total phenolic and monomeric anthocyanins by UV-Vis methods**; Nihari D Perera¹; Bonnie Rogers¹; Andrew L. Thomas¹; Michael Greenlieff¹; ¹University of Missouri-Columbia, Columbia, MO
- TP 504 **Therapeutic applications of semi-synthetic analogs derived from newly discovered variants of the antifungal occidiofungin**; Nopakorn Hansanant¹; Ravi Orugunt²; James Leif Smith^{1,2}; ¹Texas A&M University, College Station, TX; ²Sano Chemicals, Bryan, TX
- TP 505 **Application of molecular network in the differentiation of metabolic profiles of actinobacteria**; Talita Carla de Tralia Medeiros¹; Luiz Alberto Beraldo De Moraes¹; ¹Universidade de São Paulo, Ribeirão Preto, Brazil
- TP 506 **Biophysical characterisation of DNA triplexes for antigene technology**; Jack Klose¹; Alexander Begbie¹; Tara L Pukala¹; ¹University of Adelaide, Adelaide, Australia
- TP 507 **Determination of molecular weight of small interfering nucleotides siRNA by LCMS**; Jia Zheng¹; Xia Qiao Liu¹; Yuan Hong Hao¹; Hong Tao Huang¹; ¹Shimadzu(China)Co.,Ltd, Shanghai, China
- TP 508 **Information-rich spectral libraries from nucleobases and deoxynucleosides facilitate the identification of ribonucleosides by nLC-MSMS**; Guadalupe Espadas¹; Eduard Sabidó¹; ¹Proteomics Unit, Center for Genomic Regulation, Universitat Pompeu Fabra, Barcelona, Spain
- TP 509 **Flavonoid Derivatives: A Novel Triplex-Binding Ligand**; Landy Gu¹; Vanessa M. Rangel¹; Nghia Tran¹; Douglas Chu¹; Liang Xue¹; ¹University of the Pacific, Stockton, CA
- TP 510 **Human RNase 4 improves mRNA sequence characterization by LC-MS/MS**; Eric Wolf¹; Sebastian Grünberg¹; S. Hong Chan¹; Nan Dai¹; Tien-Hao Chen¹; Erbay Yigit¹; Ivan R Correa Jr.¹; ¹New England Biolabs, Inc., Beverly, MA
- TP 511 **Accelerating Oligonucleotide Research Using Novel Bioinert LC, QTOF and TQ LC-MS**; Mridul Mandal¹; Brian Domanski¹; Xiaomeng Xia¹; Nivesh Mittal¹; ¹Shimadzu Scientific Instrument, Columbia, Maryland
- TP 512 **tRNAs and tRNA modifications correlated to metastasis in melanoma via LC-MS and tRNA-seq analysis**; Cassandra Herbert¹; Balasubrahmanyam Addepalli¹; Patrick A. Limbach¹; ¹University of Cincinnati, Cincinnati, OH
- TP 513 **In-Source CID of Modified Oligonucleotides Analyzed by IP-RP LCMS: Effects of Experimental Parameters**; Stilianos G. Roussis¹; Claus Rentel¹; ¹Ionis Pharmaceuticals, Inc., Carlsbad, CA
- TP 514 **Molecular weight confirmation and impurity analysis of a 70-mer oligonucleotide**; Remco Van Soest¹; Sahana Mollah²; Kerstin Pohl³; Ling Huang⁴; ¹SCIEX, Redwood City, CA; ²Sciex, Redwood City, CA; ³Sciex, Framingham, MA; ⁴Integrated DNA Technologies, Coralville, IA
- TP 515 **OligoDistiller: An MS-platform agnostic software tool developed particularly for MS data analysis of complex**

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- oligonucleotide samples and their impurities;** Youzhong Liu¹; Piotr Probstko²; Dirk Valkenburg²; Jennifer L Lippens¹; Ronald De Vries¹; Thomas De Vijlder¹; ¹Janssen Pharmaceutica NV, Beerse, Belgium; ²Hasselt University, Hasselt, Belgium
- TP 516 **Competitive Transcription and Adduct Bypass Assay for Examining Transcriptional Perturbations and Repair of O2-Alkylthymidine Lesions;** Chen Wang¹; Xiaomei He¹; Yinan Wang¹; Yinsheng Wang¹; ¹UCR, Riverside, CA
- TP 517 **Direct chemical characterization of double-stranded oligonucleotides crosslinked by the microbiome-derived genotoxin colibactin by high-resolution mass spectrometry;** Chiara Lecchi¹; Erik S. Carlson²; Peter W. Villalta¹; Emily P. Balskus²; Silvia Balbo^{1,3}; ¹Masonic Cancer Center, University of Minnesota, Minneapolis, MN; ²Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA; ³School of Public Health, University of Minnesota, Minneapolis, MN
- TP 518 **Microflow liquid chromatography – nanoelectrospray mass spectrometry of oligonucleotides;** Guilherme Jendiroba Guimaraes¹; Franklin E Leach III¹; Michael G Bartlett¹; ¹University of Georgia, Athens, GA
- TP 519 **Tandem mass spectrometry quantification of Oligonucleotides using an isobaric internal standard;** Christopher Gawlig¹; Güngör Hanci¹; Michael Ruehl¹; ¹BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany
- TP 520 **Localization of phosphorothioate linkages in partially phosphorothioated oligonucleotides;** Samuel P Wein¹; Trenton M Peters-Clarke²; Oliver Kohlbacher³; ¹University of Tübingen, Tübingen, Germany; ²University of Wisconsin, Madison, WI; ³University of Tübingen, Tübingen, Germany
- TP 521 **Fast acquisition of DDA-MS/MS of oligonucleotides and the novel spectral merging algorithm for better assignment of sequence information;** Kosuke Uchiyama¹; Yoshihiro Kunimura¹; Simon Ashton²; Richard Price²; Helen Jose²; Atsuhiko Toyama¹; Neil Loftus²; ¹SHIMADZU Corporation, Kyoto, Japan; ²Shimadzu, Manchester, UK, Manchester, United Kingdom
- TP 522 **Profiling small oligonucleotide synthesis impurities and large mRNA sequence confirmation, including poly A and capping, using a single LC-HRMS platform;** Geert Van Raemdonck¹; Kristina Wicht¹; Jessika Wynendaele¹; Eddy Ruijter¹; Koen Iterbeke¹; ¹AnaBioTec, Evergem, Belgium
- TP 523 **Concerted application of ion mobility and tandem mass spectrometry to differentiate isomeric/isobaric oligonucleotides produced by nuclease digestion of large RNAs;** Thomas Kenderdine¹; Daniele Rollo¹; Daniele Fabris^{1,2}; ¹University of Connecticut, Storrs, CT; ²RiboDynamics LLC, Manchester, Connecticut
- TP 524 **Extending the Concept of Spectral Accuracy to the Deconvolution of Multiply Charged Large Molecules;** Yongdong Wang¹; Stacey Simonoff¹; Don Kuehl¹; Nan Zhang²; Qingfei Zheng²; ¹Cerno Bioscience, Las Vegas, NV; ²Department of Radiation Oncology, College of Medicine, Columbus, Ohio 43210
- TP 525 **Characterization of Nucleic Acid Fragment Ions by Isotopic Distributions;** Michael B Lanzillotti¹; Jessica G Pauling¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- TP 526 **LC-MS Method for Detection of Metabolites and Impurities of 1st, 2nd and 3rd Generation Oligonucleotide Therapeutics;** Irina Slobodchikova¹; Wei Lu¹; ¹Alliance Pharma, Malvern, PA
- TP 527 **The use of liquid chromatography, ion mobility, and mass spectrometry to thoroughly characterize the diastereomer composition in oligonucleotide therapeutics;** Anh Tran¹; Steven Fletcher¹; Jace W Jones¹; ¹University of Maryland, School of Pharmacy, Baltimore, MD
- TP 528 **High Temperature Fluoroalcohol-free Liquid Chromatography-Electron Detachment Dissociation Tandem Mass Spectrometry of RNA;** Carson W Szot¹; Kristina Hakansson²; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan, Ann Arbor, Michigan
- TP 529 **An oligonucleotide impurity analysis workflow with the new software that calculates percentage impurity based on summed XIC peak area;** Noriko Kato¹; Kosuke Uchiyama¹; Hiroyuki Yasuda¹; Simon Ashton²; Richard Price²; Helen Jose²; Neil Loftus²; Kiyoshi Kakiya³; Atsuhiko Toyama¹; ¹SHIMADZU Corporation, Kyoto, Japan; ²Shimadzu Corporation, Manchester, United Kingdom; ³Peptistar Inc., Settsu, Japan
- TP 530 **Optimized Fragmentation of Oligonucleotides Suppresses Undesired Fragmentation Products and Enables Confident Sequence Assignment;** Joshua Hinkle¹; William M. McGee²; Joshua P. Salem³; Robert L Ross⁴; Christopher Mullen¹; Scott Kronewitter²; John E.P. Syka¹; James L. Stephenson²; ¹Thermo Fisher Scientific, San Jose, California; ²Thermo Fisher Scientific, Lexington, Massachusetts; ³University of Michigan Ann-Arbor, Ann Arbor, MI; ⁴Thermo Fisher Scientific, Franklin, MA
- TP 531 **Investigating the role of HIV-1 genomic RNA transcriptional start site differences on Gag binding using native mass spectrometry;** Kaylee Grabarkewitz^{1,2,3}; Vicki H Wysocki^{1,2,3}; Karin Musier-Forsyth^{1,2,4}; ¹The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; ²Center for RNA Biology, The Ohio State University, Columbus, OH; ³Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; ⁴The Center for Retroviral Research, The Ohio State University, Columbus, OH
- TP 532 **Continuing the investigation of microchip capillary electrophoresis coupled with mass spectrometry in the bottom-up characterization of progressively larger RNAs;** Daniele Rollo¹; Adi Kulkarni²; Kate Yu²; Hampus Engstroem²; Guillaume Tremintin³; Daniele Fabris¹; ¹University of Connecticut, Storrs, CT; ²908 Devices, Boston, MA; ³Bruker Scientific LLC, San Jose, CA
- TP 533 **An algorithm for automated characterization of ribonuclease-digested messenger RNA using data-independent tandem mass spectrometry data;** Yuki Matsubara¹; Yasuto Yokoi¹; Jonathan Fox²; Maissa Gaye³; Joe Fredette³; Matthew A Lauber³; Guillaume Bechade²; Masami Koike⁴; Yuko Nobe⁵; Masato Taoka⁵; Hiroshi Nakayama⁴; ¹Mitsui knowledge, Minato, Japan; ²Waters S.A.S, Saint-Quentin, France; ³Waters Corporation, Milford, MA; ⁴RIKEN Center for Sustainable Resource Science, Wako, Japan; ⁵Tokyo Metropolitan University, Hachioji, Japan
- TP 534 **Metabolite Profiling and Identification of Oligonucleotide in In Vitro Metabolic System;** Gengyao Qin¹; Qiandan Miao¹; Liqi Shi¹; Zhiyu Li¹; Weiqun Cao¹; Yi Tao¹; Liang Shen¹; ¹WuXi AppTec, Shanghai, China
- TP 535 **Multiple binding and binding specificity: Lessons learned from native top-down MS of aminoglycoside/RNA complexes with different secondary structure motifs;** Sarah Viola Heel¹; Kathrin Breuker²; ¹Institute of Organic Chemistry and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, Austria; ²Institute of Organic Chemistry and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, Austria
- TP 536 **Importance of fragmentation data for the identification of phosphoramidite impurities;** Sven Hackbusch¹; Gary Held²; Kenton Chodara²; Syed K Raza²; Yi Zhang¹; Min Du³; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Milwaukee, WI; ³Thermo Fisher Scientific, Franklin, MA
- TP 537 **Fractionation of complex RNA mixtures for LC-MS/MS;** Jennifer Kist¹; Cassandra Herbert¹; Patrick Limbach¹; ¹University of Cincinnati, Cincinnati, OH

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- TP 538 **High-Resolution Accurate Mass Orbitrap mRNA Analysis: Poly-A Tail, Capping Analysis, and Bottom-up Sequence Mapping**; Alice Guo¹; Kevin Kun Guo¹; ¹*Avice Laboratories, Acton, Massachusetts*
- TP 539 **A method for predicting the monoisotopic mass in high-resolution mass spectra of oligonucleotides**; Piotr Prostko¹; Youzhong Liu²; Thomas De Vijlder²; Tatsiana Khamiakova²; Dirk Valkenborg¹; ¹*Hasselt University, Hasselt, Belgium*; ²*Janssen Pharmaceutica NV, Beerse, Belgium*
- TP 540 **A software package for sequence confirmation and impurity characterisation of synthetic oligonucleotides using MS/MS and MSE.**; Christopher Knowles¹; Jo-Anne Riley²; Jonathan Fox²; Catalin E Doneanu³; Ying Qing Yu³; ¹*Waters Corporation, Newcastle upon Tyne, United Kingdom*; ²*Waters Corporation, Wilmslow, United Kingdom*; ³*Waters corp, milford, MA*
- TP 541 **A workflow of liquid chromatography-tandem mass spectrometry data analysis for the characterization of mRNA therapeutics**; Hiroshi Nakayama¹; Masami Koike¹; Yuko Nobe²; Masato Taoka²; ¹*RIKEN Center for Sustainable Resource Science, Wako, Japan*; ²*Tokyo Metropolitan University, Hachioji, Japan*
- TP 542 **Targeted Profiling of F-Box proteome for biology and translational research**; Vijaya Pandey¹; Adarsh K Mayank²; James A Wohlschlegel²; ¹*UCLA, LOS ANGELES, CA*; ²*UCLA, Los Angeles, CA*
- TP 543 **Assessment and prediction of the human proteotypic peptide stability for proteomics quantification**; Cristina Chiva^{1,2}; Zahra Elhamraoui^{1,2}; Amanda Solé^{1,2}; Marc Serret^{1,2}; Mathias Wilhelm³; Eduard Sabidó^{1,2}; ¹*Universitat Pompeu Fabra, Barcelona, Spain*; ²*Center for Genomics Regulation, Barcelona Institute of Science and Technology (BIST), Barcelona, Spain*; ³*Technical University of Munich, Munich, Germany*
- TP 544 **Fast screening and characterization of therapeutic peptide by online capillary electrophoresis - mass spectrometry (CE-MS)**; Fuxing Xu¹; Ling Ling¹; Chuan-Fan Ding¹; Liang Wang²; Kate Yu³; ¹*Ningbo University, Ningbo, China*; ²*908 Devices, Shanghai, China*; ³*908 Devices, Boston, MA*
- TP 545 **An Ultra-Sensitive and High-Throughput Assay to Quantify Novel Bispecific Peptide by SPE-UPLC-MS/MS in Human Plasma**; Andy (hongfang) Xue¹; Pengliang Ren²; Yu Yang¹; Ruiling Wang²; Aihua Liu¹; ¹*Alliance Pharma, Malvern, PA*; ²*Shaanxi Micot Technology, Xi'an New Area, China*
- TP 546 **Integrated calibration curve-based absolute quantification of samples in SpectroDive**; Veronique Laforte¹; Maik Müller¹; Magdalena Domitrz¹; Tejas Gandhi¹; Lukas Reiter¹; ¹*Biognosys AG, Schlieren, Switzerland*
- TP 547 **A Robust Protein Normalization Strategy for Comparing Protein Expression Levels Across Tissues and Species by PRM**; Joshua Nicklav¹; Jingjing Deng¹; Eugene Ciccimaro¹; Petia Shipkova¹; ¹*Bristol-Myers Squibb, Princeton, NJ*
- TP 548 **The Proteomes that Feed the World**; Gian Luca Corongiu¹; Sarah Brajkovic¹; Patrick Roehrl¹; Andrea Piller¹; Sebastian Urzinger¹; Lukas Wuerstl¹; Paula Andrade Galan¹; Guido Giordano¹; Veronica Ramirez¹; Ezgi Aydin¹; Genc Haljiti¹; Mario Picciani¹; Qussai Abbas¹; Cemil Can Saylan¹; Armin Soleymaniniya¹; Jiuyue Pan¹; Sophia Hein¹; Corinna Dawid¹; Stephanie Heinzlmeir¹; Claus Schwechheimer¹; Chris Schoen¹; Viktoriya Avramova¹; Josch Pauling¹; Christina Ludwig¹; Dmitrij Frishman¹; Mathias Wilhelm¹; Caroline Gutjahr¹; Ralph Hueckelhoven¹; Brigitte Poppenberger¹; Bernhard Kuster¹; ¹*Elite Network of Bavaria, School of Life Sciences, Technical University of Munich, Freising, Germany*
- TP 549 **Quantitative Target Occupancy in FFPE Tissues using Immunoaffinity Capture 2D-LC-MS/MS**; Aiyng Yu¹; Lingyao Meng¹; Jintang He¹; Surinder Kaur¹; Keyang Xu¹; ¹*Genentech Inc., South San Francisco, CA*
- TP 550 **Building high-throughput analytical methods for monitoring peptide biomarkers in equine athletes**; Cecily R Wood¹; Abigail Burrows Franco¹; Alison Porter¹; Scott M Peterman²; Scott D Stanley¹; ¹*University of Kentucky, Lexington, KY*; ²*Thermo Fisher Scientific, San Jose, CA*
- TP 551 **A Robust Method for Simultaneous Detection Glycopeptide Compounds in Rat Plasma Containing Human IgG**; Li Gao¹; Na Li¹; Yanfu Ren¹; Zhiyu Li²; Lili Xing²; Yi Tao²; Liang Shen²; ¹*WuXi AppTec, Suzhou, China*; ²*WuXi AppTec, Shanghai, China*
- TP 552 **Optimizing lower limits of quantification and detection by choosing transitions in Skyline**; Nicholas Shulman¹; Lilian Heil¹; Philip M Remes²; Michael J. MacCoss¹; ¹*Department of Genome Sciences, University of Washington, Seattle, WA*; ²*Thermo Fisher Scientific, San Jose, CA*
- TP 553 **Comparison of Endogenous Peptide Quantitation Strategies**; Elena V Romanova¹; David C Platt^{2,3}; Joseph M. Williams⁴; David L. Cedeño^{3,4}; Ricardo Vallejo^{3,4}; Jonathan V. Sweedler⁵; ¹*University of Illinois at Urbana-Champaign, Urbana, IL*; ²*Illinois Wesleyan University, Bloomington, IL*; ³*SGX Medical, Bloomington, IL*; ⁴*Illinois Wesleyan University, Bloomington, Illinois*; ⁵*University of Illinois Urbana Champaign, Urbana, IL*
- TP 554 **N-Rich: A Tailored pyridine carboxaldehyde enrichment for high coverage and specificity N-terminal proteomics**; Alexandra C. Turmon¹; Andrew Palmer¹; Alexander W. Sun¹; Lisa Boatner¹; Kerian M. Backus¹; ¹*University of California, Los Angeles, Los Angeles, CA*
- TP 555 **Systematic Evaluation and Optimization of PRM Assays for the Quantification of Very Low Abundant Proteins Within Complex Samples**; Danilo Ritz¹; Christian Schori¹; Emmanuelle Lezan²; Alexander Schmidt¹; ¹*Proteomics Core Facility, University of Basel, Basel, Switzerland*; ²*Roche Innovation Center Basel, Basel, Switzerland*
- TP 556 **Targeted proteogenomics for detection of disease-associated protein isoforms - a case study of TPM2and bone mineral density**; Micah Lehe¹; Erin Jeffery¹; Abdullah Abood¹; Charles Farber¹; Gloria Sheynkman¹; ¹*University of Virginia, Charlottesville, VA*
- TP 557 **Discovery and targeted proteomic evaluation of biological responses to an MDM2 degrader in a lymphoblastic leukemia cell line**; Sarah A. Martinez¹; Eric Kuhn¹; Susanne B. Breitkopf¹; Yogesh Chutake¹; Jessica Filiatrault¹; Min Yuan¹; Yatao Shi¹; Dirk M. Walther¹; Dapeng Chen¹; Brad Enerson¹; Stefanie Schalm¹; Joyoti Dey¹; Alice McDonald¹; Matt Weiss¹; Juliet Williams¹; Chris De Savi¹; Kirti Sharma¹; ¹*Kymera Therapeutics, Inc, Watertown, MA*
- TP 558 **Multiplexed, Attomole-Level Detection of Proteotypic Peptides Associated with Retinoid Metabolism and Signaling, Using a Custom Internal-Standard Triggered SureQuantTM assay**; Robert N. O'Meally¹; Peter M. Abadir¹; Robert N. Cole¹; Brian Foster¹; ¹*Johns Hopkins School of Medicine, Baltimore, MD*
- TP 559 **Quality profiling of Tetracosactide injections using HPLC-HRMS**; Janez Ilaš¹; Aleksandra Bračko²; ¹*Faculty of Pharmacy University of Ljubljana, Ljubljana, Slovenia*; ²*Maribor University Medical Centre, Maribor, Slovenia*
- TP 560 **Development of a PRM Assay for Bona Fide Substrates of Protein Kinase CK2**; Daniel Menyhart¹; Laszlo Gyenis¹; Kristina Jurcic¹; David W Litchfield¹; ¹*University of Western Ontario, London, ON*
- TP 561 **Ocular tissue distribution and systemic pharmacokinetics of a biotherapeutic protein**; Emily Werth¹; Lin-Zhi Chen¹; ¹*Boehringer Ingelheim, Ridgefield, CT*
- TP 562 **A novel approach for generation of retention time - molecular mass chromatograms for improving**

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- interpretation and quantification of biotherapeutic molecules; Martin Green¹; Keith Richardson¹; Mark Wrona²; Yun Alelyunas²; Steve Bajic¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters Corporation, Milford, MA
- TP 563 **Assessment of Therapeutic Humanized IgG2 Antibody Concentrations in Human Plasma Using LC/PRM-MS and ELISA: A Comparative Study;** Pradyumn Maheshwari¹; Robert Popp¹; Christoph H. Borchers^{2,3,4,5}; ¹MRM Proteomics Inc., Montréal, QC; ²Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ³Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁴Division of Experimental Medicine, McGill University, Montreal, QC; ⁵Department of Pathology, McGill University, Montreal, QC
- TP 564 **Development of an Immunocapture LC-MS/MS Assay for Semi-quantitation of ADA Isotypes of a Drug in Human Serum;** Yilin Feng¹; Daniel Wall¹; Jennifer Cunliffe¹; Manisha Saxena²; Charlie G. Knutson¹; Robert Dodge³; Elena Fernandez⁴; ¹Novartis Institutes for Biomed. Research, Inc., Cambridge, MA; ²Novartis Pharma AG, Basel, Switzerland; ³Novartis Pharmaceuticals, East Hanover, New Jersey; ⁴Molecular Partners AG, CH-8952, Switzerland
- TP 565 **Quantification of anti-infliximab antibodies in human serum using capillary electrophoresis – tandem mass spectrometry;** Tessa Reinert^{1,2}; Pascal Houzé^{2,3}; Oscar Hernandez Alba⁴; Sarah Cianferani⁴; Rabah Gahoual²; Yannis Nicolas Francois⁵; ¹Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, France; ²Unité de Technologies Chimiques et Biologiques pour la Santé (UTCBS), CNRS UMR8258, Inserm U1022, Université de Paris, France; ³Laboratoire de Toxicologie Biologique, Hôpital Lariboisière, Assistance Publique – Hôpitaux de Paris (AP-HP), France; ⁴Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO) IPHC UMR 7178, Université de Strasbourg, France; ⁵Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, Strasbourg, France
- TP 566 **High throughput quantification of biologics PTM state by peptide mapping using refocussing chromatography and ZenoTOF mass spectrometry;** Moritz Heusel¹; Stephen Lock²; Nick Morrice²; Sibylle Heidelberger²; Jakob Bunkenborg¹; Michael Barrett Andersen¹; Nicolai Bache¹; ¹Evosep Biosystems, Odense, Denmark; ²SCIEX, Macclesfield, United Kingdom
- TP 567 **Advances in Intact Protein Quantitation using Gábor Transform-Based Tools in iFAMS;** Kayd L. Meldrum¹; Andrew K. Swansiger¹; Meghan M. Daniels¹; Crystal Kirmiz Cody²; Wendi A. Hale²; David L. Wong²; Michael D. Knierman²; Xi Qiu²; John Sausen²; James S. Prell^{1,3}; ¹University of Oregon, Department of Chemistry and Biochemistry, Eugene, OR; ²Agilent Technologies, Inc., Santa Clara, CA; ³Materials Science Institute, University of Oregon, Eugene, OR
- TP 568 **Development of Quantitative cGMP Impurity Protein Assays Supporting Diverse Modalities, Part II: Analysis;** Chelsea M Desbiens¹; Gustavo H M F Souza¹; Michael J Nold¹; ¹KBI Biopharma, Durham, NC
- TP 569 **Development of Quantitative cGMP Impurity Protein Assays Supporting Diverse Modalities, Part I: Discovery;** Gustavo H M F Souza¹; Chelsea M Desbiens¹; Michael J Nold¹; ¹KBI Biopharma, Durham, NC
- TP 570 **Investigating Intra- and Extra-Cellular Protein Expression to Troubleshoot Low Expression of a Challenging Biotherapeutic using Mass Spectrometry Assays;** Elsa Gorre¹; Lauren M Kraft²; Chris Sauer²; Alexander N Barnakov²; Andrew Mahan²; Thomas Kelly²; Hirsh Nanda²; Partha Chowdhury²; ¹Janssen Research and Development, Spring House, PA; ²Johnson & Johnson, Spring House, PA
- TP 571 **New USP Standards and Tools to Support Mass Spectrometry Based Multi-Attribute Method (MAM) for Therapeutics Proteins;** Li Jing¹; Jingzhong Guo¹; Kevin Carrick¹; Diane McCarthy¹; ¹USP, Rockville, MD
- TP 572 **Host Cell Proteins (HCPs) Results Analyzed using the Orbitrap Exploris 240 and Compared to Results from Gold-Standard ELISA Method;** Rodney Bannwart¹; Neelanjan Bose¹; ¹Emery Pharma, Alameda, CA
- TP 573 **Multiplex quantitation of critical host cell proteins(HCPs) using a SureQuant mass spectrometry assay peptide panel;** Jae Choi¹; Bhavin Patel¹; Terry Hicks²; Matthew Daniels²; Sarah Baron³; Km Shams Ud Doha³; Paul Gulde³; Scott M Peterman⁴; Nikki Jarrett¹; Kay Opperman¹; Ryan Bomgardner¹; ¹Thermo Fisher Scientific, Rockford, IL; ²Thermo Fisher Scientific, St Louis, MO; ³Thermo Fisher Scientific, Grand Island, NY; ⁴Thermo Fisher Scientific, San Jose, CA
- TP 574 **Size Exclusion Chromatography Coupled to Multiangle Light Scattering and High-Resolution Mass Spectrometry for the Characterization of Therapeutic Monoclonal Antibodies;** Roxana Eggleston-Rangel¹; Zeshan G Aqeel¹; ¹Phenomenex, Torrance, CA
- TP 575 **Automated Data Analysis Workflow Leveraging PASEF Data Accelerates Confident Detection of Low-Abundance HCPs;** Amy Claydon¹; Guillaume Tremintin²; Juergen Kastler³; Stuart Pengelley⁴; Jonathan Krieger²; Arnd Brandenburg³; ¹Genedata Ltd, Cambridge, United Kingdom; ²Bruker, San Jose, CA; ³Genedata AG, Basel, Switzerland; ⁴Bruker Daltonics, Bremen, Germany
- TP 576 **Peptide Characterization and Monitoring Workflow for Biosimilar mAb Drug Products using a Compliance Ready LC-MS and Informatics Platform;** Ying-Qing Yu¹; Kellen Delaney¹; Samantha Ippoliti¹; Robert E. Birdsall¹; ¹Waters Corporation, Milford, MA
- TP 577 **Structural MS of G protein-coupled receptors (GPCRs): Can HDX-MS provide sufficient information to identify ligand binding sites?;** Krzysztof Okrasa¹; Jana Broecker¹; Anna Cooper¹; Aneta Dębicka¹; Maria Serrano-Vega¹; Nicolae Solcan¹; Stacey Southall¹; ¹Sosei Heptares, Cambridge, United Kingdom
- TP 578 **Combining native mass spectrometry and mass photometry for the pentameric bacterial ligand-gated ion channel Glic;** Jérôme Castel^{1,2}; Marie Prevost³; Nathalie Barilone³; Korantin Le Mouë⁴; Manuela Zoonens⁴; Pierre-Jean Corringier³; Sarah Cianferani^{1,2}; ¹Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO), Université de Strasbourg, CNRS, IPHC, UMR 7178, Strasbourg, France; ²Infrastructure Nationale de Protéomique ProFI, FR2048 CNRS CEA, Strasbourg, France; ³Channel-Receptors Unit, Institut Pasteur, CNRS, UMR 3571, Paris, France; ⁴Laboratoire de Biologie Physico-Chimique des Protéines Membranaires, CNRS, UMR 7099, Université Paris-7, Institut de Biologie Physico-Chimique, Paris, France
- TP 579 **Capillary Zone Electrophoresis Mass Spectrometry for Characterization of Membrane Proteins;** Qianjie Wang¹; Peter K Lundquist²; Liangliang Sun¹; ¹Michigan State University, EAST LANSING; ²Michigan State University, East Lansing, MI
- TP 580 **Direct determination of membrane protein-lipid organization using lipid vesicle native mass spectrometry platform and its application in synaptic vesicle fusion;** Aniruddha Panda^{1,2}; Kallol Gupta^{1,2}; ¹Nanobiology Institute, Yale University, West Haven, Connecticut; ²Department of Cell Biology, Yale University School of Medicine, New Haven, Connecticut
- TP 581 **Analysis of lipid transport mechanisms via native mass spectrometry;** Tobias Rath¹; Rene Zangl¹; Nils Hellwig¹;

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- TP 582 **Deciphering multi drug resistance protein1 lipid trafficking using native mass spectrometry top-down approach;** Maya Miller¹; Tarick El-Baba¹; Carol V Robinson¹; ¹*Oxford University, Oxford, United Kingdom*
- TP 583 **Native mass spectrometry of extracellular vesicles to enhance understanding of molecular mechanisms in the brain;** Hannah M. Britt^{1,2}; Tarick J. El-Baba^{1,2}; Corinne A. Lutomski^{1,2}; Josh Hinkle³; Christopher Mullen³; John E.P. Syka³; Carol V. Robinson^{1,2}; ¹*Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom*; ²*Kavli Institute for NanoScience Discovery, University of Oxford, Oxford, United Kingdom*; ³*Thermo Fisher Scientific, San Jose, California*
- TP 584 **Using Native Mass Spectrometry to Probe Mechanisms of Lipid Modulation of Ion Channel Function;** Susanne M Mesoy^{1,2}; Mehtab S Hayre^{1,3}; Karin E J Rödström⁴; Stephen J Tucker^{1,5,6}; Carol V Robinson^{1,2}; ¹*Kavli Institute for Nanoscience Discovery, Oxford, United Kingdom*; ²*Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom*; ³*Medical Sciences Doctoral Training Centre, Oxford, United Kingdom*; ⁴*Centre for Medicines Discovery, University of Oxford, Oxford, United Kingdom*; ⁵*Clarendon Laboratory, Department of Physics, University of Oxford, Oxford, United Kingdom*; ⁶*OXION Initiative in Ion Channels and Disease, University of Oxford, Oxford, United Kingdom*
- TP 585 **Determining the membrane recruitment mechanisms of peripheral membrane proteins through direct top-down nativeMS analysis from a tunable lipid bilayer;** Rachel A McAllister^{1,2}; Wonhyeuk Jung¹; Kyowon Jeong³; Jared Shaw⁴; Moitrayee Bhattacharyya²; Kallol Gupta¹; ¹*Yale School of Medicine, Department of Cell Biology, New Haven, CT*; ²*Yale School of Medicine, Department of Pharmacology, New Haven, CT*; ³*Department of Applied Bioinformatics, University of Tübingen, Tübingen, Germany*; ⁴*eMSion-inc, Corvallis, OR*
- TP 586 **Development of a quantitative targeted proteomics method for the investigation of proteins in the blood-brain barrier;** Michelle Robinson¹; Carmen Fernandez-Metzler²; Serge Zemerov²; Richard King²; Tanvi Desai¹; Michael Lyman¹; Jessica Peters¹; Christopher Gibson¹; Weixun Wang¹; ¹*Merck Research Labs, West Point, PA*; ²*PharmaCadence Analytical Services, LLC, Hatfield, PA*
- TP 587 **Integrating mass spectrometry with molecular dynamics simulations for modelling IRMPD fragmentation of membrane proteins;** Neha V. Kalmankar^{1,2}; Corinne Lutomski^{1,2}; Tarick El-Baba^{1,2}; Joshua D Hinkle³; Idir Liko⁴; Jack L Bennett^{1,2}; Andrew Dolan^{1,2}; Christopher Mullen³; John E.P. Syka³; Carol V Robinson^{1,2}; ¹*Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom*; ²*Kavli Institute for NanoScience Discovery, University of Oxford, Oxford, United Kingdom*; ³*Thermo Fisher Scientific, San Jose, California*; ⁴*OMass Therapeutics, Oxford, United Kingdom*
- TP 588 **A comparative analysis of different sample preparation methods for human plasma proteomics by LC-MS/MS;** Carina Lima¹; Maggy Lepine¹; Lekha Sleno¹; ¹*University of Quebec in Montreal, Montreal, QC*
- TP 589 **Mag-Net: Bead based capture of membrane particles from plasma enables liquid biopsy measurements for >4,500 proteins;** Christine C Wu¹; Jea Park¹; Gennifer Merrihew¹; Kristine Tsantilas¹; Ireshyn Govender²; Sindisiwe Buthelezi³; Justin Jordaan²; Stoyan Stoychev²; Michael J. MacCoss¹; ¹*University of Washington, Seattle, WA*; ²*ReSyn BioSciences, Pretoria, South Africa*; ³*Council for scientific and industrial research, Pretoria, South Africa*
- TP 590 **Electron Capture Charge Reduction Allows for Selection of Individual Nanodisc Species;** Philip Lacey¹; Marius M. Kostelic¹; Sophie R. Harvey^{1,2}; Vicki H. Wysocki^{1,3}; ¹*The Ohio State University, Columbus, OH*; ²*Campus Chemical Instrumentation Center, The Ohio State University, OH, United States, Columbus, OH*; ³*Campus Chemical Instrumentation Center, The Ohio State University, Columbus, OH*
- TP 591 **Biochemical Implications of the TMEM97/ Histatin-1 Interaction;** Dominick Pierre-Jacques¹; Kyung-No Son²; Dhara Shah¹; Sang Min Lee²; Vinay Kumar Aakalu²; Stephanie M Cologna¹; ¹*University of Illinois at Chicago, Chicago, IL*; ²*University of Michigan, Ann Arbor, Michigan*
- TP 592 **Detection of Membrane Proteome Variants by Data-independent Acquisition Mass Spectrometry Approach;** Yu-Teng Jheng¹; San-Yuan Wang²; Ya-Hsuan Chang³; Hsuan-Yu Chen³; Chia-Li Han²; ¹*National Taiwan University, Taipei, Taiwan*; ²*Taipei Medical University, Taipei, Taiwan*; ³*Academia Sinica, Taipei, Taiwan*
- TP 593 **Quantitative profiling of systems-level protease activities by a mass spectrometry-cleavable signature ion-based strategy;** Fnu Ashima¹; Han Le¹; Saiful Chowdhury¹; ¹*University of Texas at Arlington, Arlington, TX*
- TP 594 **In-depth comparative proteomic analysis of human and porcine erythrocytes for the development of transfusable xeno-RBCs;** Myung Jin Oh^{1,2}; Dontan Yin^{1,2}; Jaeho Kim^{1,2}; Hyun Joo An^{1,2}; ¹*Graduate School of Analytical Science and Technology, Chungnam National University, South Korea*; ²*Asia-Pacific Glycomics Reference Site, CNU, South Korea*
- TP 595 **Characterizing the color of intact protein therapeutics by imaged capillary isoelectric focusing (icIEF)-UV/MS and peptide mapping;** Kristen Nields¹; Scott Mack²; Robert Hepler³; Andrew Mahan³; Chelsea Leonce³; Mariam Elnaggar²; Maggie Ostrowski²; Hirsh Nanda³; ¹*Janssen Biopharmaceuticals, Springhouse, PA*; ²*SCIEX, CA, USA*; ³*Janssen Pharmaceuticals, Spring House, PA*
- TP 596 **Characterization of the post translational modifications of the transcription factor EB (TFEB) and quantitation mTOR induced changes to TFEB PTMs;** Meggie N. Young¹; Karl F. Poncha¹; Nicolas L. Young^{1,2,3}; ¹*Verna and Marrs McLean Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX*; ²*Department of Molecular and Cellular Biology, Baylor College of Medicine, Houston, TX*; ³*Center for Precision Environmental Health, Baylor College of Medicine, Houston, TX*
- TP 597 **Identification of Protein Modifications Induced in E. coli Strains with a Reduced Repertoire of Anti-Oxidation Defense Enzymes by Mass Spectrometry;** Yanjia Zhang¹; Sanjay Kumar Rohaan²; James A. Imlay²; Aaron Timperman¹; ¹*University of Pennsylvania, Philadelphia, PA*; ²*University of Illinois Urbana Champaign, Urbana, IL*
- TP 598 **The potential role of SAMT247 small molecule on covalent modification of SARS-CoV-2 protein and inhibiting its function;** Tapan K. Maity¹; Jerry C. Dinan¹; Stewart R. Durell¹; Andrew J. Perciaccante¹; Daniel H. Appella²; Lisa M. Jenkins¹; ¹*Laboratory of Cell Biology, Center for Cancer Research, National Cancer Institute, Bethesda, MD*; ²*Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD*
- TP 599 **Exploration of Histone Methyltransferase Activity in the Green Alga Chlamydomonas Reinhardtii by Biochemical and Mass Spectrometry Approaches;** Emily K Wright¹; Michael Hayes¹; James Pesavento¹; ¹*Saint Mary's College of California, Moraga, CA*
- TP 600 **Temporal Responses of Skeletal Muscle Thiol Redox Proteome to Endurance Exercise Training in Six-month-old Rats;** Nicholas Day¹; Xiaolu Li¹; Matthew J Gaffrey¹; James Sanford¹; Tyler Sagendorf¹; Kwame Attah¹; Sue Bodine²; Joshua Adkins¹; Weijun Qian¹; ¹*Pacific*

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- Northwest National Laboratory, Richland, WA; ²Oklahoma Medical Research Foundation, Oklahoma City, OK
- TP 601 **Optimization of a diaPASEF method for phosphoproteomics analysis of mouse brain tissues;** Marie Gebelin¹; Christine Schaeffer¹; Jeewan Babu Rijal¹; Christine Carapito¹; ¹Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien (UMR 7178), Strasbourg, France
- TP 602 **Application of proteomic approach to identify antibody chemical liabilities in early-stage discovery;** Xiaohua Liu¹; Sagar Kathuria¹; Joel Bucci¹; Kyle Cole¹; Pierrick Rival²; Bailin Zhang¹; Alessandro Masiero²; ¹Sanofi, Cambridge, MA; ²Sanofi, Vitry-sur-Seine, France
- TP 603 **Investigating the post-translational regulation of tardigrade cryptobiosis;** Evan R. Stair¹; Abel A. Salas¹; Leslie M. Hicks¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC
- TP 604 **Acyl-Trap, a suspension trapping-based method for proteomic analysis of S-acylation;** Michael T Forrester¹; Aleksandra Tata¹; Purushothama Rao Tata¹; Matthew W Foster¹; ¹Duke University Medical Center, Durham, NC
- TP 605 **Development of a streamlined single-injection workflow for middle-down analysis of protein therapeutics using electron activated dissociation (EAD);** Haichuan Liu¹; Roxana McCloskey¹; Zoe Zhang¹; ¹SCIEX, Framingham, MA
- TP 606 **A novel role for ERp46 in platelet function revealed by IodoTMT & LC-MS/MS/MS;** Junsong Zhou¹; Tong Liu²; Yi Wu³; Hong Li²; David W. Essex³; ¹Columbia University, New York, NY; ²Rutgers New Jersey Medical School, Newark, NJ; ³Sol Sherry Thrombosis Research Center, Temple University School of Medicine, Philadelphia, PA
- TP 607 **Identification of glycosylated peptides using similarity of MS/MS spectrum;** Hyejin Kim¹; Heeyoun Hwang²; Insung Yong¹; Pilnam Kim¹; Jin Young Kim²; ¹Department of Bio and Brain Engineering, KAIST, Daejeon, South Korea; ²Korea Basic Science Institute, Ochang, South Korea
- TP 608 **SP3-RAC/IMAC: Towards Universal Proteomics Sample Processing for Multi-PTM Profiling;** Austin Gluth^{1,2}; Matthew J Gaffrey²; Xiaolu Li²; Bin Yang¹; Wei-Jun Qian²; Tong Zhang²; ¹Department of Biological Systems Engineering, Washington State University, Richland, WA; ²Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA
- TP 609 **Quality Assessment of Cellular Therapies by Structure-Based N-Glycan Mapping;** Sol Kim^{1,2}; Jihyeon Nam^{1,2}; Myungjin Oh^{1,2}; Hyun Joo An^{1,2}; ¹Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; ²Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea
- TP 610 **Disulfide bonds mapping in proteins and fluorescence-assisted quantification of cysteinyl side chains;** Sharel Cornelius¹; Christine Sarai Urbina¹; Jocelyn Vincent¹; Saiful Chowdhury¹; ¹University of Texas at Arlington, Arlington, TX
- TP 611 **Characterization of Histone Proteoforms with Capillary Electrophoresis-Tandem Mass Spectrometry using 193 nm Ultraviolet Photodissociation;** Fiza M Tajdin¹; Amanda Helms¹; Jennifer S. Brodbelt¹; ¹University of Texas, Austin, Texas
- TP 612 **Proteomic and N-Glycomic Profiling of Plasma-Derived Extracellular Vesicle and Non-Membranous Particle Subpopulations Utilizing Two-Dimensional Size Exclusion Chromatography;** Alan J. Zimmerman¹; Yunfan Gao¹; Anne-Lise Marie¹; Jacqueline Wood¹; Alexander R. Ivanov¹; ¹Barnett Institute of Chemical and Biological Analysis, Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA
- TP 613 **TimsTof DDA-PASEF phosphoproteomics analysis of human dendritic cells reveals the signaling pathways modulated by the immunosuppressive biogenic amine 3-hydroxy-L-kynurenamine (3HKA);** Cristina C Clement¹; Rajesh K Soni²; ¹Weill Cornell Medicine, New York, NY; ²Proteomics and Macromolecular Crystallography Shared Resource, Herbert Irving Comprehensive Cancer Center, Columbia University Irving Medical Center, New York, NY, United States, New York, NY
- TP 614 **Phosphoproteomics of MNT-1 Melanoma Cells Reveals Novel Signaling Pathways for Polymyxin B-induced Skin Hyperpigmentation;** Chuhan Zhang¹; Xiaofen Liu¹; Jing Zhang¹; Hailan Wu¹; Yu Wang¹; Yaxin Fan¹; Beining Guo¹; Xingchen Bian¹; Xin Li¹; ¹Institute of Antibiotics, Huashan Hospital, Fudan University, Shanghai, China
- TP 615 **Label free and Isobaric labeling mass spectrometry to monitor ubiquitination dynamics upon modulation by small molecule inhibitors;** Jeroen AA Demmers¹; Karel Bezstarosti¹; Wouter AS Doff¹; Lennart Van Der Wal¹; Karen A Sap¹; ¹Erasmus Medical Center Rotterdam, Rotterdam, Netherlands
- TP 616 **Effects of Cold Ischemia on Post-translational Modifications in Patient-Derived Xenograft Models of Cancer;** Keith D. Rivera¹; Rajan A. Burt¹; Valentina Cesarani²; Natalie M. Clark¹; D. R. Mani¹; Jean-Philippe Theurillat²; Namrata D. Udeshi¹; Steven A. Carr¹; ¹Broad Institute, Cambridge, MA; ²Institute of Oncology Research, Bellinzona, Switzerland
- TP 617 **Precision characterization of Phosphorylations Enabled by Individual Ion Mass Spectrometry in MEK1 protein;** Raveena Gupta¹; Bryon Drown¹; Jared O. Kafader¹; John P. McGee¹; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL
- TP 618 **Tackling citrullination and deamidation challenges in proteomics using high-resolution ion mobility-mass spectrometry (HRIM-MS);** Heidi Vitrac¹; Jordan Stewart¹; Lauren Royer¹; Ashli Simone¹; Jesse Meyer²; Justyna Fert-Bober²; Jennifer Van Eyk²; ¹MOBILion Systems, Chadds Ford, PA; ²Cedars-Sinai Medical Center, Los Angeles, CA
- TP 619 **A proximity labeling-based orthogonal trap approach for identifying the spatiotemporal posttranslational modifications-network regulated by enzymes in living cells;** Guijin Zhai¹; Yepei Huang¹; Kai Zhang¹; ¹Tianjin Medical University, Tianjin, China
- TP 620 **Co-Translational Incorporation of Non-Canonical Proline Analogues in Bacteria: a Novel Approach to Study the Chromatography of Modified Peptides in LC-MS;** Alexandre J.J Prefontaine¹; Ying Lao¹; Victor Spicer¹; Darien Yeung¹; Nediljko Budisa¹; Oleg V. Krokhin¹; ¹University of Manitoba, Winnipeg, MB
- TP 621 **Orthogonal methods quantify a proteomic profile associated with AKT inhibitor response in both breast cancer cell lines and patient tumors;** Constance Sobsey^{1,2}; Bjoern C Froehlich³; Georgia Mitsa^{1,2}; Arif Awan⁴; Adriana Aguilar-Mahecha⁵; Mark Basik^{5,6}; Christoph H Borchers^{1,4,6}; Gerald Batist^{4,7}; ¹Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, Montreal, QC; ²Division of Experimental Medicine, McGill University, Montreal, QC; ³CeMOS - Center for Mass Spectrometry and Optical Spectroscopy, Mannheim, Germany; ⁴Gerald Bronfman Department of Oncology, McGill University, Montreal, QC; ⁵Segal Cancer Centre, Lady Davis Institute, Jewish General Hospital, Montréal, QC; ⁶MRM Proteomics Inc., Montréal, QC; ⁷Exactis Innovation, Montreal, QC
- TP 622 **Comprehensive proteome landscape of low- and high-grade gliomas;** Chunyan Lan; Peking Union Medical College, Beijing, China
- TP 623 **Utilization of a disposable tip-based LC system for proteomic characterization of FFPE tissues and plasma-derived extracellular vesicles from TNBC patients;** Vincent R. Richard^{1,2}; Georgia Mitsa^{1,3}; Yasamin Majedi²; Josiane Lafleur²; Adriana Aguilar-Mahecha²; Rodney Ouellette⁴; Jeremy Roy⁴; Mark Basik^{2,5,6}; Christoph H. Borchers^{1,3,7,8}; ¹Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ²Lady Davis

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- Institute for Medical Research, Jewish General Hospital, Montreal, QC; ³Division of Experimental Medicine, McGill University, Montreal, QC; ⁴Atlantic Cancer Research Institute, Moncton, NB; ⁵Department of Surgery, McGill University, Montreal, QC; ⁶Department of Oncology, McGill University, Montreal, QC; ⁷Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ⁸Department of Pathology, McGill University, Montreal, QC
- TP 624 **Determination of a biomarkers panel to predict the response to treatment with dexamethasone for Sars-Cov2 / COVID-19 pneumonia; Jerome Vialaret¹; Christophe Hirtz¹; Jana Kindermans¹; Margaux Vignon¹; Erika Nogue²; Nicolas Molinari²; Clement Boissin²; Jeremy Charriot²; ¹Montpellier Hospital, Proteomics platform (PPC), Montpellier, France; ²Montpellier Hospital, Clinical Research and Epidemiology Unit, Montpellier, France**
- TP 625 **Quantitative Proteomics of Human Retinal Pigment Epithelium (RPE) Using Chimerys-UHR-IonStar Enabled In-Depth Exploration of Age-Related Macular Degeneration (AMD) Pathology; Shichen Shen¹; Ming Zhang¹; Shuo Qian²; Sandra R. Montezuma³; Deborah A. Ferrington⁴; Jun Qu^{1,5}; ¹University at Buffalo, Buffalo, NY; ²Roswell Park Comprehensive Cancer Center, Buffalo, NY; ³University of Minnesota, Minneapolis, MN; ⁴Doheny Eye Institute, Pasadena, CA; ⁵New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY**
- TP 626 **Automated sample preparation for bottom-up urinary proteome profiling in clinical proteomics; Ireshyn S Govender^{1,2}; Previn Naicker²; Andrea Ellero³; Rethabile Mokoena^{2,4}; Justin Jordaani¹; Stoyan Stoychev¹; ¹ReSyn Biosciences, Pretoria, South Africa; ²Council for scientific and industrial research, Pretoria, South Africa; ³University of Pretoria, Pretoria, South Africa; ⁴University of the Witwatersrand, Johannesburg, South Africa**
- TP 627 **Dual viscosity mixture vehicle for intratympanic steroid treatment modifies the ROS and inflammation related proteomes; Jinwoo Jung^{1,2}; Hyeyoon Kim^{1,2}; Eunji Jeon^{1,2}; Hui Li³; Junghun Lee³; Yujung Hwang³; Kisoon Dan¹; Myungwhan Suh³; Mookyun Park³; Dohyun Han^{1,2}; ¹Proteomics Core Facility, Transdisciplinary Research and Collaboration, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; ²Transdisciplinary Department of Medicine and Advanced Technology, Seoul National University Hospital, Seoul, South Korea; ³Department of Otorhinolaryngology-Head and Neck Surgery, Seoul National University Hospital, Seoul, South Korea**
- TP 628 **Proteomics application in discovering therapeutic effect of dental mesenchymal stem cell secretome on stroke; Sehoon Park¹; Kyung-Joo Seong²; Se Hwan Jang¹; Daseul Kim¹; Ji-Yeon Jung²; Won-Jae Kim²; Zee-Yong Park¹; ¹School of Life Science, Gwangju Institute of Science and Technology, Cheomdangwagi123, Buk-gu, Gwangju, South Korea; ²Dental Science Research Institute, Stem cell Secretome Research Center, Hard-tissue Biointerface Research Center, Department of Oral Physiology, School of Dentistry, Chonnam National University, Gwangju, South Korea**
- TP 629 **Quantification of intra-amniotic inflammation in late preterm prelabor rupture of membranes associated with the response of amniotic fluid proteome; Marie Vajrychova¹; Jaroslav Stráňík¹; Rudolf Kupčík¹; Rudolf Kukla³; Radka Bolehovská³; Marian Kacerovský²; ¹Biomedical Research Center, University Hospital Hradec Kralove, Hradec Kralove, Czech Republic; ²Department of Obstetrics and Gynecology, University Hospital Hradec Kralove and Faculty of Medicine in Hradec Kralove, Charles University, Hradec Kralove, Czech Republic; ³Institute of Clinical Microbiology, University Hospital Hradec Kralove, Hradec Kralove, Czech Republic**
- TP 630 **Quantification of the PD-1/PD-L1 axis in non-small cell lung cancer by immuno-multiple reaction monitoring; Vincent Lacasse^{1,2}; Rene P. Zahedi^{3,4,5}; Vincent R, Richard¹; Hangjun Wang²; Georgia Mitsa¹; Olivier Poetz⁶; Margaret Redpath²; Andreas Papadakis²; Mounib Elchebly²; Victor Cohen⁷; Jason Scott Agulnik⁷; Gerald Batist⁷; Alan Spatz^{2,7}; Christoph H. Borchers^{1,2,7,8}; ¹Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ²Department of Pathology, McGill University, Montreal, QC; ³Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; ⁴Department of Internal Medicine, University of Manitoba, Winnipeg, MB; ⁵Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; ⁶Signatope GmbH, Reutlingen, Germany; ⁷Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ⁸Division of Experimental Medicine, McGill University, Montreal, QC**
- TP 631 **Proteomic predictors of colon tumor distant metastasis; Anna Wojakowska¹; Lukasz Marczak²; Marcin Zeman³; Marta Gawin³; Lukasz Skoczylas³; Katarzyna Dubkiewicz²; Mykola Chekan⁴; Ewa Zembala-Nozynska³; Monika Anna Pietrowska³; ¹Institute of Bioorganic Chemistry Polish Academy of Sciences, Poznan, Poland; ²Institute of Bioorganic Chemistry Polish Academy of Sciences, Poznan, Poland; ³Maria Skłodowska-Curie National Research Institute of Oncology, Gliwice Branch, Gliwice, Poland; ⁴Academy of Silesia, Katowice, Poland**
- TP 632 **Evaluation of an unbiased, deep, and scalable multi nanoparticle-based proteomics workflow for limited plasma sample volume from model organisms; Shao-Yung Chen¹; Lucy Williamson¹; Margaret Donovan¹; Purvi Tandel¹; Gabriel Castro¹; Taher Elgierari¹; Aaron S Gajadhar¹; ¹Seer, Redwood City, CA**
- TP 633 **Development and qualification of a novel high throughput DIA LC-MS/MS method to enable clinical fecal biomarker discovery; Ellen Casavant¹; Brandon Harder¹; Manuel Magana¹; Magdalena Bober²; Jakob Vowinkel²; W. Rodney Mathews¹; Veronica Anania¹; ¹Genentech, South San Francisco, CA; ²Biognosys AG, Schlieren, Switzerland**
- TP 634 **Automating dwell time determination to increase the efficiency of highly multiplexed SRM method refinement; Scott Peterman¹; Alan Atkins²; Martin Jech³; Abigail Burrows Franco⁴; Scott D Stanley⁴; Neloni Wijeratne⁵; ¹Thermo Fisher Scientific, Fort Walton Beach, FL; ²ThermoFisher Scientific, Hemel Hempstead, United Kingdom; ³Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; ⁴University of Kentucky, Lexington, KY; ⁵Thermo Fisher Scientific, San Jose, CA**
- TP 635 **DIA method optimization for large-scale urinary proteomics discovery studies on an Easy-nLC™ coupled to Q-Exactive HF-X; Manubhai Kadavil Prabhakaran^{1,2}; Dijana Vitko³; Shannon Dimartino^{1,2}; Ted Lee^{1,2}; Amy Chan^{1,2}; Candace Chung^{1,2}; Jayme Leschly^{1,2}; Emily Morrison^{1,2}; Richard S Lee^{1,2}; John Froehlich^{1,2}; ¹Boston Childrens Hospital, Boston, MA; ²Harvard Medical School, Boston, MA; ³PrognomiQ Inc, San Mateo, CA**
- TP 636 **Integrative proteome analysis for discovery of potential CAR-NK target in TNBC; Sunghyun Huh¹; Yourae Shin¹; Ji Eun Park¹; Gangsoo Jung¹; Unbeom Kang¹; ¹Bertis R&D Division, Bertis Inc., Seongnam-si, South Korea**
- TP 637 **Investigating the risk of relapse in non-small cell lung cancer with proteomics; Corinna Friedrich^{1,2}; Simon Schallenberg²; Gabriel Dernbach²; Philipp Keyl^{2,3}; Mohamed Hajji¹; Matthias Ziehm^{1,2}; Sylvia Niquet^{1,2}; Christin Beier¹; Frederick Klauschen^{2,3}; Philipp Mertins¹; ¹MDC Berlin, Berlin, Germany; ²Charité – Universitätsmedizin Berlin, Berlin, Germany; ³Ludwig-Maximilians-Universität München, Munich, Germany**

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- TP 638 **Deeper plasma proteome coverage enables identification of novel biomarkers and classification of diseases;** Andreas Schmidt¹; Katrin Hartinger²; Zehan Hu²; Claudia Martelli³; Katharina Limm²; Xaver Wurzenberger²; Sebastian Mueller⁴; Nils A. Kulak²; ¹*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*; ²*PreOmics GmbH, Planegg/Martinsried, Germany*; ³*Bruker Switzerland AG, Fällanden, Switzerland*; ⁴*Biognosys AG, Zurich, Switzerland*
- TP 639 **Integrative Proteomics and Pharmacological Analysis of Colon Cancer Reveals the Classical Lipogenic Pathway with Prognostic and Therapeutic Opportunities;** Abhilash Barpanda¹; Sanjeeva Srivastava¹; ¹*IIT Bombay, Mumbai, India*
- TP 640 **diaPASEF proteomic analysis of human sputum samples for the early diagnosis of lung cancer;** Alejandro Fernández-Vega¹; María Del Sol Arenas-De Larriva²; Bernabé Jurado-Gómez²; Ignacio Ortea³; ¹*Institute for Biomedical Research and Innovation of Cadiz, Cadiz, Spain*; ²*Pneumology Unit, Hospital Universitario Reina Sofia, IMIBIC. University of Cordoba, Cordoba, Spain*; ³*Proteomics Unit, Nanomaterials and Nanotechnology Research Center (CINN-CSIC), Health Research Institute of Asturias (ISPA), Oviedo, Spain*
- TP 641 **Quantification of human milk protein survival across the infant gastrointestinal tract using nano LC/Orbitrap MS;** Brianne Waj¹; Ningjian Liang¹; Bum Jin Kim¹; Brian Scottoline²; David Dallas¹; ¹*Oregon State University, Corvallis, OR*; ²*Oregon Health & Science University, Portland, Oregon*
- TP 642 **Next-generation biotyping of microorganisms for assessment of antibiotics resistance and virulence factors;** Allan Stensballe¹; Nicolai Bache²; Dorte Bekker-Jensen²; Mads Lause Mogensen³; ¹*Aalborg University, Aalborg, Denmark*; ²*Evosep Biosystems, Odense, Denmark*; ³*Treat Systems, Aalborg, Denmark*
- TP 643 **Ultra-deep proteome profiling of Alzheimer's disease cerebrospinal fluid by data-independent acquisition mass spectrometry using long gradients and ion mobility separation;** Ellen Casavant¹; Sumedh Sankhe²; Jakob Vowinckel³; Nikhil Pandya²; Meena Choi²; Cecilia Monteiro²; W. Rodney Mathews²; Veronica Anania²; ¹*Genentech, South San Francisco, CA*; ²*Genentech Inc, South San Francisco, CA*; ³*Biognosys AG, Zurich, Switzerland*
- TP 644 **Proteogenomic Landscape of East-Asian Breast Cancer Reveals Pathogenesis and Subtypes for Prognostic and Therapeutic opportunities;** Ya-Hsuan Chang¹; Yi-Ju Chen²; Zhi-Jie Hong³; Yi-Jing Hsiao⁴; Guo-Shiou Liao³; Sheng-Fang Su⁵; Kuen-Tyng Lin²; Huei-Wen Chen⁶; Yen-Shen Lu^{7, 8}; Hsuan-Yu Chen¹; Sung-Liang Yu⁴; Jyh-Cherng Yu³; Yu-Ju Chen²; ¹*Institute of Statistical Science, Academia Sinica, Taipei, Taiwan*; ²*Institute of Chemistry, Academia Sinica, Taipei, Taiwan*; ³*Department of Surgery, Tri-Service General Hospital, National Defense Medical Center, Taipei, Taiwan*; ⁴*Department of Clinical Laboratory Sciences and Medical Biotechnology, College of Medicine, National Taiwan University, Taipei, Taiwan*; ⁵*Graduate Institute of Oncology, National Taiwan University College of Medicine, Taipei, Taiwan*; ⁶*Graduate Institute of Toxicology, National Taiwan University College of Medicine, Taipei, Taiwan*; ⁷*Department of Medical Oncology, National Taiwan University Hospital, Cancer Center Branch, Taipei, Taiwan*; ⁸*Department of Oncology, National Taiwan University Hospital, Taipei, Taiwan*
- TP 645 **Deep plasma protein profiling with a novel fully automated multi-nanoparticle-based sample preparation and high throughput data-independent acquisition LC-MS method;** William F Beimers¹; Noah M Lancaster²; Evgenia Shishkova¹; Sterling C Johnson^{3, 4, 5}; Joshua J. Coon^{1, 2, 6}; ¹*Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI*; ²*Department of Chemistry, University of Wisconsin -*
- Madison, Madison, WI*; ³*Department of Medicine, University of Wisconsin-Madison, Madison, WI*; ⁴*Wisconsin Alzheimer's Institute, University of Wisconsin-Madison, Madison, WI*; ⁵*Wisconsin Alzheimer's Disease Research Center, University of Wisconsin School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*; ⁶*Morgridge Institute for Research, Madison, WI*
- TP 646 **Charge-Based Fractionation of Blood Plasma-Derived Extracellular Vesicle Subpopulations Followed by Proteomic Characterization;** Xianyi Su¹; Alexander R. Ivanov¹; ¹*Barnett Institute of Chemical and Biological Analysis, Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA*
- TP 647 **Detecting low abundance hepatic factor to elucidate pulmonary arteriovenous malformations in congenital heart disease through comparative human serum proteomic analysis;** Laura Yuriko González-Teshima¹; Maiko Okamura²; Takashi Nirasawa³; Keisuke Hakamada¹; Tadashi Ikeda¹; Kozue Murata^{1, 4}; Kenji Minatoya¹; Hidetoshi Masumoto^{1, 4}; Masaya Ikegawa²; ¹*Department of Cardiovascular Surgery, Graduate School of Medicine, Kyoto University, Kyoto-city, Japan*; ²*Department of Life and Medical Systems, Doshisha University, Kyotanabe-city, Japan*; ³*Bruker Japan K.K., Yokohama, Japan*; ⁴*Clinical Translational Research Program, RIKEN Center for Biosystems Dynamics Research, Kobe, Japan*
- TP 648 **The Proteome Changes in Human Periodontal Ligament and Pulp Fibroblasts Resulting from Contact with Root Restorative and Pulp-capping Materials;** Mona Goli¹; Mahmoud Mona²; Firas Kobeissy³; Roberta Pileggi²; Yehia Mechref¹; ¹*Texas Tech University, Lubbock, TX*; ²*University of Florida College of Dentistry, Gainesville, FL*; ³*Morehouse School of Medicine (MSM), Atlanta, Georgia*
- TP 649 **The Antitumor Effect of the DNA Polymerase Alpha Inhibitor ST1926 on Protein Expression in Glioblastoma;** Waziha Purba¹; Mona Goli¹; Chirine El-Baba²; Zeinab Ayache²; Zeinab Kawtharani²; Berthe Hayar²; Claudio Pisano³; Firas Kobeissy^{2, 4}; Nadine Darwiche²; Yehia Mechref¹; ¹*Texas Tech University, Lubbock, Texas*; ²*American University of Beirut, Beirut, Lebanon*; ³*Biogem, Research Institute, Ariano Irpino, Italy*; ⁴*Morehouse School of Medicine (MSM), Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Atlanta, Georgia*
- TP 650 **Development of Extracellular vesicles preparation platform for clinical proteomics;** Satoshi Muraoka¹; Masayo Hirano¹; Satoshi Nagayama²; Junko Isoyama¹; Mimiko Ishida¹; Takeshi Tomonaga¹; Jun Adachi^{1, 3}; ¹*National Institute of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan*; ²*The Cancer Institute Hospital of the Japanese Foundation for Cancer Research, Ariake, Japan*; ³*Kyoto University, Kyoto, Japan*
- TP 651 **Blood Stream Isolates: What's in a Proteome?;** Morgan Hepburn¹; Mario E Valdes-Tresanco¹; Rory Gilliland¹; Anika Westlund¹; Annegret Ulke-Lemee¹; Soren Wacker¹; Alikhan Mansuri¹; Gopal Ramamourthy¹; Thomas Rydzak¹; Joshua T Smith²; Andriy Plakhotnyk¹; Colin MacKenzie¹; Maryam Mapar¹; Bruce J Walker²; Ashlee M Earl²; Hallgrimur Benediktsson¹; Daniel B Gregson¹; M. Ethan McDonald¹; Ian A Lewis¹; ¹*University of Calgary, Calgary, AB*; ²*Broad Institute, Cambridge, MA*
- TP 652 **Early Inflammatory Protein Responses Detected in Plasma by MALDI-ToF Profiling in SARS-CoV-2 Immunization Naïve Individuals;** Amanda Weaver¹; Tristan Finch¹; Alicia Patrick¹; Laura Peek¹; Gary Pestano¹; ¹*Biodesix, Boulder, CO*
- TP 653 **The Role of Native MS in Antibody Research Against Snake Envenoming;** Irina Oganesyan¹; Julian A. Harrison²; Ledsgaard Jensen Line³; Cecilie Knudsen^{3, 4}; Timothy Patrick Jenkins³; Andreas H. Laustsen-Kiel^{3, 4}; Renato Zenobi²; ¹*ETHZ, Zürich, Switzerland*; ²*ETH Zurich, Zurich, Switzerland*; ³*Technical University of Denmark, Kongens*

TUESDAY POSTERS

- Lyngby, Denmark; ⁴VenomAid Diagnostics ApS, Kongens Lyngby, Denmark
- TP 654 **Capillary chromatographic separation of nanogram protein quantities on a wide-pore superficially porous particle column for top-down proteomics**; Guillaume Chevreux¹; Laurent Lignieres¹; Véronique Legros¹; Manel Khelil¹; Nicolas Senecaut¹; Matthew A Lauber²; Jean-Michel Camadro¹; ¹Institut Jacques Monod, PARIS, France; ²Waters Corporation, Milford, MA
- TP 655 **Can precursor ion connectivity of different isolation windows improve peptide and protein identification in chimeric MS/MS spectra?**; Lily R Adair¹; Ian Jones²; Rainer Cramer¹; ¹Department of Chemistry, University of Reading, Reading, United Kingdom; ²School of Biological Sciences, University of Reading, Reading, United Kingdom
- TP 656 **Improved characterization of ApoA4 proteoforms from plasma samples by top-down mass spectrometry using ion-ion reactions and advanced spectral averaging**; Amal Mohamed Kamal¹; Jake T Kline¹; Kenneth R Durbin²; Konstantin O Nagornov³; Yury O Tsybin³; Luca Fornelli¹; ¹University of Oklahoma, Norman, OK; ²Proteinaceous, Evanston, Illinois; ³Spectroswiss, Lausanne, Switzerland
- TP 657 **FLASHDeconvQ: a software tool for proteome-wide label-free quantification of proteoforms in top-down proteomics**; Jihyung Kim¹; Kyowon Jeong¹; Konrad Winkels²; Philipp T. Kaulich²; Andreas Tholey²; Oliver Kohlbacher¹; ¹University of Tübingen, Tübingen, Germany; ²Christian-Albrechts-Universität zu Kiel, Kiel, Germany
- TP 658 **FLASHIda:deep - Historically informed data acquisition in top-down LC-MS/MS batch runs**; Kyowon Jeong¹; Philipp T. Kaulich²; Konrad Winkels²; Jihyung Kim¹; Andreas Tholey²; Oliver Kohlbacher¹; ¹University of Tübingen, Tübingen, Germany; ²Christian-Albrechts-Universität zu Kiel, Kiel, Germany
- TP 659 **A new proteomics data analysis software for top-down mass spectrometry**; George Alevizos¹; Mariangela Kosmopoulou¹; Athanasios Smyrnakis¹; Dimitris Papanastasiou¹; ¹Fasmatech, NCSR Demokritos, Athens, Greece
- TP 660 **VUV photodissociation using a diffuse light source integrated in the Omnitrap platform**; Athanasios Smyrnakis¹; Mariangela Kosmopoulou¹; Dimitris Papanastasiou¹; ¹Fasmatech, NCSR Demokritos, Athens, Greece
- TP 661 **False discovery rate estimation in spectral deconvolution in top-down proteomics**; Ayesha Feroz¹; Kyowon Jeong^{1,2}; Konstantin Nagornov³; Jihyung Kim^{1,2}; Timo Sachsenberg^{1,2}; Yury O. Tsybin³; Oliver Kohlbacher^{1,2,4}; ¹Applied Bioinformatics, Department for Computer Science, University of Tübingen, Sand 14, 72076, Tübingen, Germany; ²Institute for Bioinformatics and Medical Informatics, University of Tübingen, Sand 14, 72076, Tübingen, Germany; ³Spectroswiss, 1015, Lausanne, Switzerland; ⁴Translational Bioinformatics, University Hospital Tübingen, Hoppe-Seyler-Str. 9, 72076, Tübingen, Germany
- TP 662 **Protein Cooking: Combining Thermal CID and EAD for intact protein sequencing**; Cuong Le¹; Patrick Pribil¹; Yves Le Blanc²; ¹SCIEX, Concord, ON; ²SCIEX, Concord, ON, ON
- TP 663 **Capillary Zone Electrophoresis-Field Asymmetric Ion Mobility Spectrometry-Mass Spectrometry (CZE-FAIMS-MS) of Histone Protein Analysis for Top-down Proteomics**; Qianyi Wang¹; Fei Fang¹; Liangliang Sun¹; ¹Michigan State University, East Lansing, MI
- TP 664 **Combining Long-Read RNA Sequencing with Curated Databases to Enhance Proteoform Identification & Characterization by Top-Down Proteomics**; Joseph B. Greer^{1,2}; Bryan P. Early¹; Taojunfeng Su¹; Ryan T. Fellers^{1,2}; Neil L. Kelleher¹; Kenneth R. Durbin^{1,2}; ¹Northwestern University, Evanston, IL; ²Proteinaceous, Evanston, IL
- TP 665 **Top-down analysis of intact NISTmAb and CA (II) by Capillary Isoelectric Focusing coupled to Electron Capture Dissociation Mass Spectrometry**; Stanislav Beloborodov¹; Pavel Ryumin¹; Wen Jin¹; Bradley Schneider¹; Bill Lloyd²; ¹SCIEX, concord; ²SCIEX, Concord, ON
- TP 666 **Leveraging intrachain disulfide bonds in proteins for improved sequence coverage in EAD top-down analysis**; Wen Jin¹; Pavel Ryumin¹; Lyle L. Burton¹; ¹SCIEX, Concord, ON
- TP 667 **Real-Time Spectrum Generation and Online Parameter Optimization During Individual Ion Mass Spectrometry Acquisition**; Ryan T. Fellers¹; Michael A. R. Hollas¹; Bryan P. Early¹; Joseph B. Greer¹; John P. McGee¹; Kenneth R. Durbin²; Jared O. Kafader¹; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL; ²Proteinaceous, Evanston, Illinois
- TP 668 **DeepY: A deep learning model for evaluating bio-similarity of antibody drugs by intact glycoproteins analysis using LC-MS**; Jung Hoon Choi¹; Geul Bang¹; Kun Cho¹; Hyun Joo An²; Heeyoun Hwang¹; ¹Korea Basic Science Institute, Cheongjusi, South Korea; ²Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea
- TP 669 **Internal fragments generated by top-down mass-spectrometry can be confidently assigned by cyclic ion-mobility, enhancing the extent of protein sequence information**; Muhammad A Zenaidee¹; Tyren M Dodgen²; Gene Hart-Smith¹; Luke Carroll³; ¹Australian Proteome Analysis Facility, Macquarie University, Sydney, Australia; ²Waters Corporation, Sydney, Australia; ³Australian Proteome Analysis Facility, Macquarie University, Macquarie Park, Australia
- TP 670 **Internal fragmentation generates progressively smaller terminal fragments in top-down mass spectrometry**; Novera Alam¹; Somak Ray¹; Jeffrey N Agar¹; ¹Northeastern University, Boston, MA
- TP 671 **Coupling high-field asymmetric waveform ion mobility spectrometry with capillary zone electrophoresis-tandem mass spectrometry for top-down proteomics**; Tian Xu¹; Liangliang Sun¹; ¹Michigan State University, East Lansing, MI
- TP 672 **A standardized approach for the exploration of histone proteoforms with EAD fragmentation on the Sciex ZenoTOF MS**; Richard M Searfoss¹; Emily Zahn¹; Zongtao Lin¹; Francisca N. de Luna Vitorino¹; Benjamin A Garcia¹; ¹Washington University School of Medicine, St. Louis, MO
- TP 673 **Heavy peaks -examples of qualitative and quantitative potential of intact protein LC-MS**; Walteri Hosa¹; VTT Technical Research Centre of Finland, Espoo, Finland
- TP 674 **Evaluation of Spray-Capillary-Based Capillary Electrophoresis-Mass Spectrometry for Analysis of Sub-nanogram Mass Intact Complex Lysate using Top-Down Proteomics**; Zhitao Zhao¹; Yanting Guo¹; Kellye A Cupp-Sutton¹; Lushuang Huang¹; Si Wu¹; ¹Oklahoma University, Norman, OK
- TP 675 **Assessing alternative proteases for quantitative proteomics**; Meital Kupervasser¹; David Morgenstern¹; Corine Katina¹; Yishai Levin¹; ¹The De Botton Protein Profiling institute of the Nancy and Stephen Grand Israel National Center for Personalized Medicine, Weizmann Institute of Science, Rehovot, Israel
- TP 676 **Real-time instrument methods to resolve chimeric spectra and post-translational modifications in multiplexed proteomics**; Chris McGann¹; William Barshop²; Jesse Canterbury²; Chuwei Lin³; Thomas Perkins³; David Bergen²; Jingjing Huang²; Graeme McAlister²; Devin Schweppe³; ¹University of Washington, Seattle, WA; ²Thermo Fisher Scientific, San Jose, CA; ³University of Washington, Seattle, WA
- TP 677 **directLFQ, an algorithm for ultra-fast, accurate and open proteomics quantification**; Constantin Ammar¹; Julia Schessner¹; Sander Willems¹; André Michaelis¹

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- Matthias Mann¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany
- TP 678 **Proteomics reveals specific metabolic pathways responsible for the antinociceptive effect of Flavonoids found in Cannabis sativa**; Fatma Boujenoui¹; Mathilde Lahaise¹; Francis Beaudry¹; ¹Universite de Montreal, St-Hyacinthe, QC
- TP 679 **ESI Source Comparison and Optimization on a Capillary-flow SureQuant Assay**; Yi (Jimmy) Zeng¹; Ruby Karimjee¹; Sara Nouri Gomaei¹; Hao Qian¹; Esthelle Hoedt¹; Joon-Yong Lee¹; Philip Ma¹; Bruce Wilcox¹; ¹PrognomiQ Inc, San Mateo, CA
- TP 680 **Enabling high throughput proteomics with short gradients and ZenoSWATH DIA by utilising the speed and sensitivity of the ZenoToF 7600**; Dylan Xavier¹; Keith Ashman²; Peter G Hains¹; Phillip J Robinson¹; ¹ProCan®, Children's Medical Research Institute, Faculty of Medicine and Health, The University of Sydney, Westmead, Australia; ²SCIEX, Sydney, Australia
- TP 681 **High-throughput sample preparation workflow for absolute quantitative proteomics combining cell-free QconCAT synthesis and in-StageTip digestion**; Ayako Takemori¹; Ryo Konno²; Yusuke Kawashima²; Yuto Hamazaki³; Ayuko Hoshino³; Nobuaki Takemori¹; ¹Ehime University, Toon, Japan; ²Kazusa DNA Research Institute, Kisarazu, Japan; ³Tokyo Institute of Technology, Yokohama, Japan
- TP 683 **Non-invasive micro-sampling and targeted MS-based longitudinal blood proteome profiling to establish intra-individual protein reference ranges of athletes**; Vincent R, Richard¹; Georgia Mitsa^{1,2}; Daria Chaplygina¹; Mario Thevis^{3,4}; Christoph H. Borchers^{1,2,5,6}; ¹Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ²Division of Experimental Medicine, McGill University, Montreal, QC; ³Institute of Biochemistry, Center for Preventive Doping Research, German Sport University, Cologne, Germany; ⁴European Monitoring Center for Emerging Doping Agents (EuMoCEDA), Cologne/Bonn, Germany; ⁵Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ⁶Department of Pathology, McGill University, Montreal, QC
- TP 684 **Enhanced TMT data analysis with AI-driven workflows utilizing CHIMERYS and INFERYs algorithms**; Mick Greer¹; Mark Sanders²; David M Horn³; Kai Fritzscheier⁴; ¹Thermo Fisher Scientific, Austin, TX; ²ThermoFisher Scientific, Somerset, NJ; ³ThermoFisher Scientific, San Jose, CA; ⁴Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- TP 685 **Discovery and validation of "missing human proteins" based on analysis of gastric cancer tumor cells**; Yining Cai¹; Chunhui Gu¹; Fuchung Hsiao¹; Jennifer B Dennison¹; Jody Vykoukal¹; Johannes Fahrman¹; Kim-Anh Do¹; Shumei Song¹; Jaffer Ajani¹; Ehsan Irajizad¹; Hiroyuki Katayama¹; Samir Hanash¹; ¹University of Texas MD Anderson Cancer Center, Houston, TX
- TP 686 **Developing differential absolute quantification assays for targeted cancer proteogenomics**; Yassene Mohammed¹; Constantinos Blidjios²; Karl Makepeace³; Pallab Bhowmick³; Vincent R, Richard⁴; Christoph H. Borchers^{5,6,7,8}; ¹Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; ²Department of Oncology, McGill University, Montreal, QC; ³University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; ⁴Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ⁵Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁶Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ⁷Division of Experimental Medicine, McGill University, Montreal, QC; ⁸Department of Pathology, McGill University, Montreal, QC
- TP 687 **Quantitative Proteomic Analysis of Sputum Reveals Proteins Associated with Inflammatory Response to Woodsmoke Exposure**; Angie L Mordant¹; Christine A Mills¹; Alexis Payton^{2,3}; Laura E Herring¹; Neil E Alexis⁴; Heather Wells⁴; David B Peden^{4,5}; Julia Rager^{2,3,6}; Ilona Jaspers^{2,4,7}; ¹UNC Proteomics Core Facility, Department of Pharmacology, University of North Carolina at Chapel Hill, Chapel Hill, NC; ²Department of Environmental Sciences and Engineering, Gillings School of Global Public Health, UNC Chapel Hill, Chapel Hill, NC; ³Center for Environmental Medicine and Lung Biology, School of Medicine, UNC Chapel Hill, Chapel Hill, NC; ⁴Center for Environmental Medicine Asthma and Lung Biology, Department of Pediatrics, UNC Chapel Hill, Chapel Hill, NC; ⁵Department of Pediatrics, Division of Allergy & Immunology, UNC Chapel Hill, Chapel Hill, NC; ⁶Institute for Environmental Health Solutions, Gillings School of Global Public Health, UNC Chapel Hill, Chapel Hill, NC; ⁷Department of Microbiology and Immunology, UNC Chapel Hill, Chapel Hill, NC
- TP 688 **An API-independent Smart-close-out enable faster TMT RTS-SPS-MS3 assisted in-depth proteome profiling**; Weixian Deng¹; Aman Makaju¹; Daryl Bulloch²; Bo Zhou¹; ¹Amgen, Thousand Oaks, CA; ²Amgen, Inc., South San Francisco, CA
- TP 689 **Proteomic Analysis of Six Mammalian Cell Lines Reveals Individual Lysosomal Composition and Novel Lysosomal Proteins**; Sara Bonini¹; Fatema Akter¹; Sriganayatri Ponnaiyan¹; Bianca Kögler-Mohrbacher²; Florian Bleibaum³; Markus Damme³; Bernhard Y Renard²; Dominic Winter¹; ¹Institute for Biochemistry and Molecular Biology, Medical Faculty, Rheinische Friedrich-Wilhelms-University of Bonn, Bonn, Germany; ²Bioinformatics Unit (MF1), Robert Koch Institute, Berlin, Germany; ³Institute for Biochemistry, Kiel, Germany
- TP 690 **TMT quantitative proteomics of bortezomib treated cell line models of AL amyloidosis and multiple myeloma**; Gary Bradshaw¹; Cameron S Fraser^{1,2,3}; Marian Kalocsay⁴; Kristopher Sarosiek^{1,2,3}; ¹Laboratory of Systems Pharmacology, Boston, MA; ²John B. Little Center for Radiation Sciences, Harvard TH Chan School of Public Health, Boston, MA; ³Program in Molecular and Integrative Physiological Sciences, Harvard TH Chan School of Public Health, Boston, MA; ⁴Department of Experimental Radiation Oncology, Division of Radiation Oncology, The University of Texas MD Anderson Cancer Center, Houston, TX
- TP 691 **Light-dark dependent changes in cyanobacterium Crocosphaera subtropica ATCC 51142 proteome**; Punyatoya Panda¹; Uma K Aryal¹; ¹Purdue University, West Lafayette, Indiana
- TP 692 **Systemized proteomics by automating the TMT global proteome profiling workflow**; Taylor P Ma¹; Hanna G Budayeva²; Kristan Bahten³; Beibei Huang⁴; Maowei Dou³; ¹Genentech, Inc., South San Francisco, CA; ²Genentech Inc, South San Francisco, CA; ³ThermoFisher Scientific, San Jose, CA; ⁴Thermo Fisher Scientific, San Jose, CA
- TP 693 **Enabling high depth proteomic analysis of rat plasma through comparison of depletion strategies**; Jan Muntel¹; Theresa Keil¹; Christin Zasada¹; Janine Sequeira¹; Marsilio Adriani²; Krzysztof Okrasa²; Hannes Hahne¹; ¹OmicScouts, Freising, Germany; ²Sosei Heptares, Cambridge, United Kingdom
- TP 694 **Proteomic characterization of Oreochromis niloticus skin used as a biological dressing**; Iasmim Lopes De Lima¹; Cláudia B. A. Medeiros²; Isabella Cavalcanti²; Fabricio Oliveira Souto²; Marcos Nogueira Eberlin¹; Roberto Afonso Da Silva²; Marcelo Borges Miranda³; José Luiz Lima Filho²; ¹MackMass Laboratory, Mackenzie Presbyterian University, São Paulo, Brazil; ²Keizo Asami Institute,

TUESDAY POSTERS

- TP 695 **Deep proteome profiling of breast implant capsules with contracture shows high burden of inflammatory processes;** Ole Østergaard¹; Andreas Larsen²; Tim Kongsmark Weltz²; Mikkel Herly³; Jesper Velgaard Olsen¹; ¹*NNF CENTER FOR PROTEIN RESEARCH, Copenhagen, Denmark*; ²*Department of Plastic Surgery and Burns Treatment, Copenhagen University Hospital, Copenhagen, Denmark*; ³*Department of Immunology and Microbiology, University of Copenhagen, Copenhagen, Denmark*
- TP 696 **Comprehensive Proteomics Analysis of the Crustacean Cuticle;** Vu Ngoc Huong Tran¹; Gaoyuan Lu¹; Wenxin Wu²; Thao Duong²; Lingjun Li^{1,2}; ¹*University of Wisconsin-Madison School of Pharmacy - Madison, WI, Madison, WI*; ²*Department of Chemistry, University of Wisconsin-Madison, Madison, WI*
- TP 697 **Phosphoproteomic profiling of Stk33-knockout testis reveals widespread phosphorylation changes in spermatogenesis;** Weiling Yu¹; Liping Yao¹; Yang Li¹; Hong Chen¹; Chenghao Situ¹; Zhibin Hu¹; Xuejiang Guo¹; ¹*Nanjing Medical University, Nanjing, China*
- TP 698 **Kinase assay-linked phosphoproteomic profiling identified AKAP3/4 as important phosphorylation substrates of STK33 during spermiogenesis;** Chenghao Situ¹; Weiling Yu¹; Hong Chen¹; Liping Yao¹; Xiangzheng Zhang¹; Xuejiang Guo¹; ¹*Nanjing Medical University, Nanjing, China*
- TP 699 **A medium-throughput DIA-MS workflow enables pre-clinical and clinical proteome studies in cardiac tissue;** Lisa Neuenroth¹; Jumana Jaber¹; Verena Ebner¹; Stephan Lehnart^{1,2,3,4}; Henning Urlaub^{1,3,5}; Christof Lenz^{1,2,3,4,5}; ¹*University Medical Center Goettingen, Goettingen, Germany*; ²*DFG Collaborative Research Center 1002, Goettingen, Germany*; ³*DFG Collaborative Research Center 1190, Goettingen, Germany*; ⁴*DZHK, Goettingen, Germany*; ⁵*Max Planck Institute for Multidisciplinary Sciences, Goettingen, Germany*
- TP 700 **Identification of proteins affected by increased intraocular pressure in the glaucomatous female mouse retina by label-free proteomics;** Khadiza Zaman¹; Autumn B Morgan²; Vien Nguyen¹; Katalin Prokai-Tatrai¹; Denise M Inman²; Laszlo Prokai¹; ¹*Department of Pharmacology and Neuroscience, The University of North Texas Health Science Center, Fort Worth, TX*; ²*Department of Pharmaceutical Sciences and the North Texas Eye Research Institute, The University of North Texas Health Science Center, Fort Worth, TX*
- TP 701 **Optimization of Extraction Methods to Allow Detection and Quantification of Protein Targets from Various Mammalian Tissues;** Fabio N. Najjar¹; Yulanda M. Williamson²; Paul J. Branham¹; Hans C. Cooper²; John R. Barr²; Tracie L. Williams²; ¹*Oak Ridge Institute for Science and Education, Atlanta, GA*; ²*National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, GA*
- TP 702 **Comparison of Sample Preparation Methods for Genetically Variant Peptide Identification in Human Hair;** Zheng Zhang¹; William E. Wallace¹; Guanghui Wang¹; Meghan C. Burke Harris¹; Yi Liu¹; Sergey L. Sheetlin¹; Stephen E. Stein¹; ¹*NIST, Gaithersburg, MD*
- TP 703 **Spatially-resolved proteomics of drug-dosed tissue by use of liquid extraction surface analysis;** Peter Macey¹; Iain B. Styles¹; Helen J. Cooper¹; ¹*University of Birmingham, Birmingham, United Kingdom*
- TP 704 **Differential proteomics to probe molecular basis for a renal phenotype associated with GPR110 deletion;** Bill Huang¹; Karl Kevala¹; Hee-Yong Kim¹; ¹*NIAAA/NIH, Rockville, Maryland*
- TP 705 **Hollow Fiber Field-Flow Fractionation coupled with nano-LC/MS/MS improved the characterization of protein aggregates in whole brain lysates from B6 mice;** Zohaib Khan¹; Valentina Marassi²; Barbara Roda²; Cristina C. Clement¹; ¹*Weill Cornell Medicine, New York, New York*; ²*Department of Chemistry, University of Bologna, Bologna, Italy*
- TP 706 **MALDI and LC-ESI-MS for amyloid-beta peptide profiling in brain of Alzheimer's disease and Down syndrome patients;** Elena Camporesi¹; Amal Kasri²; Gunnar Brinkmalm³; Marie-Claude Potter²; Henrik Zetterberg³; Eleni Gkanatsiou¹; Lev Stimmer⁴; Andre Strydom⁵; Yannick Vermeiren⁶; ¹*Gothenburg University, Gothenburg, Sweden*; ²*Institute du Cerveau-CNRS UMR7225-Inserm U1127-UPMC, Hopital de la Pitié-Salpêtrière 47, Paris, Paris, France*; ³*University of Gothenburg, Molndal, Sweden*; ⁴*INSERM US27, Platform for Experimental Pathology, MIRCen, Fontenay-aux-Roses, France, Paris, France*; ⁵*Department of Forensic and Neurodevelopmental Sciences, Institute of Psychiatry, Psychology and Neuroscience, King's College London, London, United Kingdom, London, United Kingdom*; ⁶*Department of Biomedical Sciences, Laboratory of Neurochemistry and Behavior, Institute Born-Bunge, University of Antwerp, Wilrijk, Antwerp, Belgium, Antwerp, Belgium*
- TP 707 **Data independent acquisition generates a proteomic profile of CYLD deficient human skin tumours;** Joseph Inns¹; José Luis Marín-Rubio¹; Matthias Trost¹; Neil Rajan¹; ¹*Newcastle University, Newcastle upon Tyne, United Kingdom*
- TP 708 **A multi-enzyme protocol provides greater amino acid sequence coverage of collagen and elastin in extracellular matrices;** Leonard B Collins¹; Taufika Islam Williams¹; Andreea Biehl^{1,2}; Ana Gracioso Martins^{1,2}; Zachary Davis^{1,2}; Daphne Sze^{1,2}; Camilo Mora-Navarro³; Matthew Fisher^{1,2}; Donald Freytes^{1,2}; ¹*North Carolina State University, Raleigh, NC*; ²*University of North Carolina at Chapel Hill, Chapel Hill, NC*; ³*University of Puerto Rico, Mayaguez, Puerto Rico*
- TP 709 **Survey of Estrogen-Related Endocrine Disruption in Aquatic Ecosystems by Mass Spectrometry-Based Proteomics Using Hylella azteca as Model Organism;** Marcel L. Prokai¹; Khadiza Zaman²; Vladimir Shulaev¹; ¹*University of North Texas, Denton, TX*; ²*University of North Texas Health Science Center, Fort Worth, TX*
- TP 710 **Biting into the Tooth Proteome: protein extraction, data acquisition, and data processing;** Priyam Jani¹; Olivier Duverger¹; Marian Young¹; Lee Jannice¹; Yan Wang¹; ¹*NIH/NIDCR, BETHESDA, MD*
- TP 711 **SYSTEMS BIOLOGY OF ATHEROSCLEROTIC HUMAN CAROTID ARTERIES THROUGH MASS SPECTROMETRY-BASED PROTEOMICS;** Laszlo Prokai^{1,2}; Éva Csösz²; Gergő Kalló²; Ajnees Kumar²; Khadiza Zaman¹; Uladzislau Vadadokhau²; László Potor^{2,3}; Zoltán Hendrik²; Gábor Méhes²; Csaba Tóth²; Péter Gergely²; József Tözsér²; György Balla³; József Balla^{2,3}; ¹*University of North Texas Health Science Center, Fort Worth, TX*; ²*University of Debrecen, Faculty of Medicine, Debrecen, Hungary*; ³*University of Debrecen, ELKH-UD Vascular Pathophysiology Research Group, Debrecen, Hungary*
- TP 712 **Quantitative Target Engagement for a KRASG12C Inhibitor in FPFE Tumor Tissue;** Andrew Chambers¹; Steve Sweet¹; Zifeng Song¹; David Chain¹; Claire Rooney²; Yeoun Jin Kim¹; ¹*AstraZeneca R&D, Gaithersburg, Maryland*; ²*AstraZeneca, Cambridge, United Kingdom*
- TP 713 **Proteomics of adipose tissue-derived extracellular vesicles from bariatric surgery patients;** Jacelyn Greenwald¹; Paola Loreto Palacio²; Yongseok Kim¹; Setty M Magaña²; Vicki H Wysocki¹; ¹*The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH*; ²*Department of Pediatrics, Division of Neurology, Center for Clinical and Translational Research, Abigail Wexner Research Institute, Nationwide Children's Hospital, Columbus, Ohio*

TUESDAY POSTERS

- TP 714 **Poly[n]rotaxanes: From Synthesis To Mass Spectrometric Characterizations;** Bo Song¹; James Seale¹; Yunyan Qiu²; Fraser Stoddart¹; ¹Northwestern University, Evanston, IL; ²National University of Singapore, Singapore, Singapore
- TP 715 **Detecting Oxygen Inhibition in Adhesive Systems Using ASAP-MS;** Christopher Joseph Shaffer¹; Spencer Johnson²; Dana Reed¹; Amanda Leone¹; Wayne Mahoney¹; Eric Nelson¹; ¹3M, Saint Paul, MN; ²Brigham Young University, Provo., UT
- TP 716 **Dissecting Complex Polymer Mass Spectra by Fourier Transform-based Deconvolution and Macromolecular Mass Defect Analysis;** Andrew K Swansiger¹; Christopher M. Crittenden²; Rekha Thomas²; James S Prell^{1,3}; Bifan Chen²; ¹University of Oregon, Eugene, OR; ²Genentech Inc, South San Francisco, CA; ³Materials Science Institute, University of Oregon, Eugene, OR
- TP 717 **Investigation of fluoropolymers by Thermodesorption/Pyrolysis-DART coupled to very high-resolution mass spectrometry;** Pierre Pacholski^{1,2}; Frédéric Progent¹; Sébastien Schramm²; Frédéric Aubriet²; ¹CEA, DAM, DIF, F-91297 Arpajon, France; ²Laboratoire de Chimie et Physique-Approche Multi-échelles des Milieux Complexes (LCP-A2MC), Université de Lorraine, METZ, France
- TP 718 **Direct analysis of brominated flame retardants in high-impact polystyrene and acrylonitrile butadiene styrene copolymer with DIP-APCI Q-TOF MS;** Ville Nissinen¹; Krista Gronlund¹; Janne Janis¹; Jarkko J. Saarinen¹; Mika Suvanto¹; Ilkka Rytöluoto²; Jani Pelto²; ¹University of Eastern Finland, Department of Chemistry, Joensuu, Finland; ²VTT Technical Research Centre of Finland Ltd., Tampere, Finland
- TP 719 **Combining IMS with MS/MS for Accelerated Readout of Digital Polymers;** Isaure Sergent¹; Thibault Schutz²; Laurence Oswald³; Jean-François Lutz²; Laurence Charles¹; ¹Aix Marseille Université, CNRS, Institut de Chimie Radicalaire, MARSEILLE, France; ²Université de Strasbourg, CNRS, UMR 7006, Institut de Science et d'Ingénierie Supramoléculaires, Strasbourg, France; ³Université de Strasbourg, CNRS, UPR 22, Institut Charles Sadron, Strasbourg, France
- TP 720 **Controlling the charge states of ultra-high molecular weight polystyrene MALDI ions through cationization reagents;** Avinash Adhikrao Patil¹; Thị Khánh Ly Lại¹; Wen-Ping Peng¹; ¹National Dong Hwa University, Shoufeng, Taiwan
- TP 721 **>10,000 Da polymer detection using Q Exactive™ UHRM: In-Source Trapping and Charge Reduction;** Junho Jeon¹; Anthony Gies¹; Zoltan Szabo²; Katie Peterson²; ¹The Dow Chemical Company, Lake Jackson, TX; ²Thermo Fisher Scientific, San Jose, CA
- TP 722 **Detecting and Identifying Sample-Classification Markers from Direct-HRMS Experiments: How to Manage Comparative DART-HRMS data;** Luke K Ackerman¹; Kristen L Reese¹; Jānis Ruško²; Ingus Pērkons²; ¹FDA Center for Food Safety, College Park, MD; ²Institute of Food Safety, Animal Health and Environment "BIOR", Riga, Latvia
- TP 723 **An LC-MS/MS method for the determination of a kind of polypentose with polysulfonic groups in SD rat tissue homogenate;** Chao Liu¹; Feixue Wang¹; Li Fang¹; Peiyun An¹; Jinlian Lu¹; Zhiyu Li¹; Lili Xing¹; Yi Tao¹; Liang Shen¹; ¹WuXi AppTec, Shanghai, China
- TP 724 **Waters RADIANT™ ASAP Probe: Industrial Application of a ASAP Direct Mass Detector and a UHR-MS ASAP;** Janece Potter¹; Junho Jeon¹; Anthony Gies¹; Bryan Katzenmeyer²; ¹Dow, Inc., Lake Jackson, TX; ²Waters Corporation, Milford, MA
- TP 725 **NP-SIMS as a tool for evaluating the homogeneity of extreme-ultraviolet resists;** Jander Cruz¹; Stanislav Verkhoturov²; Emile A. Schweikert²; Michael Eller¹; ¹California State University Northridge, Northridge, CA; ²Texas A&M University, College Station, TX
- TP 726 **High throughput mass spectrometry-based metabolomics reveal nanoplastics-induced mitochondrial dysfunction in normal human-derived cells;** Lin Siyi^{1,2,3}; Zongwei Cai^{1,2}; Chunmiao Zheng^{3,4}; ¹State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, Hong Kong SAR, China, Hong Kong, China; ²Department of Chemistry, Hong Kong Baptist University, Hong Kong, China; ³State Environmental Protection Key Laboratory of Integrated Surface Water-Groundwater Pollution Control, School of Environmental Science and Engineering, Southern University of Science and Technology, Shenzhen, China; ⁴EIT Institute for Advanced Study, Ningbo, China
- TP 727 **LC-MRM Analysis Reveals Improved In Vivo Stability of SMARTag® Tandem-Cleavage MMAE Antibody-Drug Conjugates as Compared to Vedotin Conjugates;** Dominick Y Yeo¹; Reji N Nair¹; Ayodele O Ogunkoya¹; Xiao Cai¹; Stepan Chuprakov¹; Robyn M Barfield¹; Maxine Bazoun¹; Tiffany Unsulangi¹; Jesus Aguilar¹; Thomas Linz¹; Jia Yang¹; Fangjiu Zhang¹; Alyssa G Occiano¹; Dharmaraj Samuel¹; Penelope M Drake¹; ¹Catalent Pharma Solutions, Emeryville, CA
- TP 728 **Detection and quantitation of benzodiazepines in less than 3 min using Probe ElectroSpray Ionization mass spectrometry and isotope dilution approach;** Pauline Griffeuille¹; Sylvain Dulaurent¹; Souleiman El Balkhi¹; Stephane Moreau²; Franck Saint-Marcoux¹; ¹CHU Limoges, Limoges, France; ²SHIMADZU Europe, Cugnaux, France
- TP 729 **Harmful textile chemicals - Investigation of dermal uptake and peptide modifications in reconstructed human epidermis;** Josefine Carlsson¹; Pablo Pardo Menacho¹; Conny Ostman¹; Ulrika Nilsson¹; ¹Stockholm University, Stockholm, Sweden
- TP 730 **Modeling The Effect of Staphylococcal Enterotoxin B on Cardiac, Epidermal and Lung Cells Utilizing Organ-on-a-Chip Methodology;** Conor C Jenkins¹; Elizabeth Dhummakupt²; Gabrielle Rizzo²; Allison Melka³; Dylan Fudge²; Tyler Goralski²; ¹U.S. Army DEVCOM CBC, APG, MD; ²U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; ³EXCET Incorporated, Edgewood, MD
- TP 731 **Drugs of abuse in hair: high speed and sensitivity demands for LC-MS/MS;** Ichiro Hirano¹; Marcos Pudenzi²; Luis Otavio Junqueira²; ¹Shimadzu do Brasil Comercio Ltda, Barueri, Brazil; ²Shimadzu do Brasil Comercio Ltda, Barueri, Brazil
- TP 732 **An Untargeted Workflow to Comprehensively Identify Drug-Related Adducts for Bioactivation Derisking in Drug Discovery and Development;** Yu Feng¹; Ili Erdemir¹; Lei Zhu¹; Matthew Kuhls¹; Wen Kang¹; Nianyu Li¹; Raymond Gonzalez¹; Kara Pearson¹; ¹Merck & Co., West Point, PA
- TP 733 **Investigating the fate of hazardous textile pollutants in a new process for chemical recycling of post-consumer garments;** Tim Åström¹; Maria Ximena Ruiz Caldas²; Ioannis Sadiktis²; Ulrika Nilsson²; Aji P Mathew²; ¹Stockholm University, Stockholm, Sweden; ²Stockholm University, Stockholm, Sweden

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

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Cancer Research III.....	071-096
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Systems Biology.....	696-711
Viruses and Virus-Like Particles.....	712-730

- WP 001 **High Throughput Quantitative Algal Toxin Analysis by Paper Spray Ionization Tandem Mass Spectrometry (PS-MS/MS)**; Lucas R. Abruzzi^{1,2}; Daniel G. Beach³; Erik T. Krogh^{1,2,4}; Christopher G. Gill^{1,2,5,6}; 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 Washington, Seattle, WA*
- WP 002 **A New Approach for Clinical Albuminuria Diagnostics: Simultaneous Quantitation of Urinary Albumin and Creatinine by High-Throughput Paper Spray Mass Spectrometry**; Igor Pereira¹; Joseph Monaghan^{1,2}; Lucas R. Abruzzi^{1,2}; Jason L. Robinson³; Christopher G. Gill^{1,2,4,5,6}; ¹*Appl. Env. Res. Labs. (AERL), Nanaimo, BC*; ²*University of Victoria, Victoria, BC*; ³*Health PEI, Charlottetown, PEI*; ⁴*Vancouver Island University, Nanaimo, BC*; ⁵*Simon Fraser University, Burnaby, BC*; ⁶*University of Washington, Seattle, WA*
- WP 003 **Underwater Analyses of Tissue Surrogates with the Liquid Micro-junction Surface Sampling Probe (LMJ-SSP)**; Mark McKeown¹; Jian Yu¹; Richard Oleschuk¹; ¹*Queen's University, Kingston, ON*
- WP 004 **Trace and Bulk Detection of Post-Burn and Post-Blast of Energetics by 3D-Printed Cone Spray Ionization Mass Spectrometry**; Patrick W Fedick¹; Ryan M Bain²; Tj Pinedo¹; Christopher C. Mulligan³; Douglas J. Klapec²; ¹*Naval Air Warfare Center, Weapons Division, China Lake, CA*; ²*Bureau of Alcohol, Tobacco, Firearms and Explosives, Beltsville, MD*; ³*Illinois state university, Normal, IL*
- WP 005 **SPME-DART-MS Provides a Rapid Screening Tool for PFAS Analysis**; Ronald V. Emmons¹; Aghogho A. Olomukoro¹; William L. Fatigante²; Brian Musselman²; Emanuela Gionfriddo¹; ¹*The University of Toledo, Toledo, OH*; ²*Bruker Scientific, Billerica, MA*
- WP 006 **DART-TOF for Rapid Forensic Analysis of Oil Spills. What Can We Measure?**; Robert B Cody¹; Krishnaja Tikkiyetti²; Paige McCallum²; Taylor Filewood²; Jeffrey Yan²; Honoria Kwok²; Pamela Brunswick²; Dayue Shang²; ¹*JEOL USA, Inc., Peabody, MA*; ²*Pacific and Yukon Laboratory for Environmental Testing, North Vancouver, BC*
- WP 007 **Electrokinetic charging: the mechanism behind electroless ionization mass spectrometry (ELI-MS)**; Stefan Kooij¹; Cees Van Riijn¹; Neil Ribe²; Daniel Bonn¹; ¹*Van der Waals Zeeman Institute, Amsterdam, Netherlands*; ²*Lab FAST, Université Paris-Saclay, CNRS, Orsay, France*
- WP 008 **Cell line phenotype predication in real-time using automated Laser Assisted-Rapid Evaporative Ionisation Mass Spectrometry (LA-REIMS)**; Paul Abu-Rabie; GSK, Stevenage, Hertfordshire, United Kingdom
- WP 009 **Reaction acceleration in nanodrops investigated using rapid and variable mixing with theta glass emitters**; Casey J Chen¹; Evan R. Williams¹; ¹*University of California Berkeley, Berkeley, CA*
- WP 010 **Silica nanoparticles induce oxidative stress as measured by mass spectrometry**; Yangjie Li¹; Kurt W. Kolasinski²; Richard N Zare¹; ¹*Stanford University, Stanford, CA*; ²*West Chester University, West Chester, PA*
- WP 011 **Comparison of SWATH, DDA, and PRM Methods for Screening Novel Psychoactive Substances in Plasma by Paper Spray Mass Spectrometry**; Hannah Zimmerman-Federle¹; Nicholas Manicke¹; ¹*Indiana University Purdue University Indianapolis, Indianapolis, IN*
- WP 012 **PGE2 is localized outside the COX2 positive implantation site during pregnancy**; Joanne B Ballantyne¹; Thanai Paxton²; Yuri Sugiura³; Rae Maeda³; ¹*Waters, Manchester, United Kingdom*; ²*Nihon Waters, Tokyo, Japan*; ³*Graduate School of Medicine, Kyoto University, Kyoto, Japan*
- WP 013 **Electrospray ionization enhancement: phosphate as an additive to eliminate alkali metal ion adducts**; Myriam

WEDNESDAY POSTERS

- WP 014 **Interfacing LC-ESI/APCI and GC-DBDI to the same instrument: the ideal HR-MS Swiss Knife for a Mass Spectrometry Core Facility;** Natalia Gasilova¹; Daniel Trujillo Ortiz¹; Laure Menin¹; ¹EPFL SB ISIC-GE, Lausanne, Switzerland
- WP 015 **Real time volatile sulfur compounds monitoring using DART ion source;** Motoshi Sakakura¹; Teruhisa Shiota¹; Yasuhiko Bando¹; ¹AMR Inc., Meguro-Ku, Japan
- WP 016 **Polymeric Surface Modification of Swabs for Enhanced Detection of Lipids Using High Throughput DESI-MS;** Elmeri Latvanen¹; Maria Sani¹; Dani Simon¹; Alva Si¹; Yuchen Xiang¹; Vincen Wu¹; Petra Paizs¹; James Kinross¹; Panagiotis Manesiotis²; Zoltan Takats¹; Lauren Ford¹; ¹Imperial College London, London, United Kingdom; ²Queen's University Belfast, Belfast, United Kingdom
- WP 017 **Heterogeneous Catalysis by Fullerene C-60: Photocatalytic Dehydro-Dimerization of Primary Amines and Tetrahydroquinolines;** Savithra Javaraj¹; Kavyasree Chintalapudi¹; Abraham Kwame Badu-Tawiah¹; ¹The Ohio State University, Columbus, OH
- WP 018 **Temperature Profiling and Quantitative Analysis of Disperse Dyes in Polyester via DART Mass Spectrometry;** Zoe J Millbern; ¹NC State University, Raleigh, NC
- WP 019 **Rapid Identification of Double Bond Positions of Lipids in Butter by using Probe ESI Q-TOF LCMS-9050 and OAD-MS/MS;** Yohei Arai¹; Yuta Miyazaki¹; Natsuyo Asano¹; Hidenori Takahashi¹; ¹SHIMADZU Corporation, Kyoto, Japan
- WP 020 **Sensitive analysis of residual protein Tat Bh 1-101 in Lentiviral Vectors for Gene Therapy by LC-MS/MS;** Yan Lu¹; Chao-Xuan Zhang¹; Patrick Rodrigues¹; Lei Yang¹; Aaron Shafer¹; Frank Fazio¹; ¹St. Jude Children's research hospital, Memphis, TN
- WP 021 **Improved Biopharmaceutical Peptide Mapping Workflows Using a Novel Autolysis-Resistant Trypsin Enzyme;** Samantha Ippoliti¹; Nick Zampa¹; Ying Qing Yu¹; Matthew A Lauber¹; ¹Waters Corporation, Milford, MA
- WP 022 **Mass spectrometric ITEM-ONE analysis confirms and refines an assembled affimer binding site on the HER-2 targeting therapeutic antibody Pertuzumab;** Claudia Röwer¹; Oladapo Olaleye²; Rainer Bischoff²; Michael O. Glocker¹; ¹Proteome Center Rostock, Rostock, Germany; ²Department of Analytical Biochemistry, Faculty of Science & Engineering, University of Groningen, Groningen, Netherlands
- WP 023 **Advanced assessment through intact glycopeptide analysis of Infliximab's biologics and biosimilar;** Heeyoun Hwang¹; Hyejin Kim²; Geul Bang¹; Hyun Joo An³; Jong Shin Yoo¹; Jin Young Kim¹; ¹Yeseul Park⁴; ¹Korea Basic Science Institute, cheongju, South Korea; ²Korea Advanced Institute of Science and Technology, Daejeon, South Korea; ³Chungnam National University, Daejeon, South Korea; ⁴Korea Basic Science Institute, Cheongju, South Korea
- WP 024 **Ex vivo mass spectrometry-based biodistribution of total antibody and released payload of an ADC;** Domenico Ravazza¹; Lucrezia Principi¹; Lydia Bisbal Lopez²; Andrea Galbiati¹; Aureliano Zana¹; Matilde Bocchi¹; Sheila Dakhel¹; Samuele Cazzamalli¹; Dario Neri^{3,4}; Alberto Dal Corso²; Ettore Gilardoni¹; ¹Philochem AG, Otelfingen, Switzerland; ²Chemistry Department, Università degli studi di Milano, Milan, Italy; ³ETH Zurich, Zurich, Switzerland; ⁴Philogen S.p.A., Sovicelle, Italy
- WP 025 **Comparison of glycopeptide and released N-glycan abundances for IgG-based therapeutic antibodies;** Concepcion Africano Remoroza¹; Meghan C. Harris-Burke¹; Tytus D. Mak¹; Brian T. Cooper^{1,2}; Zachary C. Goecker¹; Sergey L. Sheetlin¹; Yuri A. Mirokhin¹; Guanghui Wang¹; Xiaoyu Yang¹; Dmitrii V. Tchekhovskoi¹; Stephen E. Stein¹; ¹National Institute of Standards and Technology, Gaithersburg, MD; ²University of North Carolina at Charlotte, Charlotte, North Carolina
- WP 026 **Novel LC-MS-based Platform for Extensive Investigation on Antibody-Drug Conjugates Induced Ocular Toxicity;** Xiaoyu Zhu¹; Min Ma²; Ming Zhang¹; Jun Qu^{1,3}; ¹University at Buffalo, Buffalo, NY; ²Roswell Park Comprehensive Cancer Center, Buffalo, NY; ³New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY
- WP 027 **Simultaneous antibody sequencing and epitope mapping by integrated cryo electron microscopy and mass spectrometry;** Marta Šiborová¹; Douwe Schulte¹; Joost Snijder¹; ¹Utrecht University, Utrecht, Netherlands
- WP 028 **Comprehensive Biotransformation Analysis of a DAR4 ADC using Intact LC-HRMS from in vivo Cynomolgus Monkey Samples;** Hui Yin Tan¹; Yue Huang¹; Jiaqi Yuan¹; Anton I. Rosenbaum¹; ¹AstraZeneca, South San Francisco, CA
- WP 029 **Multi-specific construct separation using native reversed-phase liquid chromatography;** Shuai Wu¹; Aniruddha Sahasrabudhe¹; Wenchao Sun¹; ¹Amgen Inc., Thousand Oaks, CA
- WP 030 **Charge heterogeneity characterization and peak identification of complex protein therapeutics using an icIEF-UV/MS system;** Mingjie Cui¹; Kristin Schultzkuszak¹; Trust Razunguzwa¹; Weiguo Zhai¹; Scott Mack²; Jingwen Ding²; Zoe Zhang²; Maggie Ostrowski²; ¹AstraZeneca, Gaithersburg, MD; ²SCIEX, Fremont, CA
- WP 031 **Paper-Based Immunoassay for Multiplexed Detection of Colorectal Cancer Biomarkers Through Direct Paper Spray Mass Spectrometry;** Girish Muralikrishnan¹; Abraham Kwame Badu-Tawiah¹; ¹The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH
- WP 032 **In-depth characterization of viral antigens using collision-induced dissociation (CID) and electron activated dissociation (EAD);** Hari Kosanam¹; George Perkins¹; Jared Kress¹; Haichuan Liu²; Eshani Nandita²; Zoe Zhang²; ¹Merck & Co., Inc., West Point, PA; ²SCIEX, Redwood city, CA
- WP 033 **Ion Mobility-Mass Spectrometry and Collision Induced Unfolding Rapidly Quantifies the Structural Dynamics of a Therapeutic Fc-Fusion Protein;** Henry W Li¹; Rosendo Villafuerte-Vega¹; Thomas R. Slaney²; Naresh Chennamsetty²; Guodong Chen²; Li Tao²; Brandon T Ruotolo¹; ¹University of Michigan, Ann Arbor, Michigan; ²Bristol Myers Squibb, New Brunswick, NJ
- WP 034 **High resolution ion mobility-mass spectrometry (HRIM-MS) for rapid gas-phase separation and characterization of peptides containing asparagine deamidations and isoaspartates (isoAsp);** Andrew B. Dykstra¹; Heidi Vitrac²; Thomas Lubinsky²; Ashli Simone²; Iain D. G. Campuzano¹; Pavel Bondarenko¹; ¹Amgen, Thousand Oaks, CA; ²MOBILion Systems, Inc., Chadds Ford, PA
- WP 035 **Probing the cause of antibody discoloration via relative quantification of glycation and associated species using an EAD-based multi-attribute methodology (MAM);** Haichuan Liu¹; Andrew Mahan²; Hirsh Nanda²; Elliott Jones¹; Zoe Zhang¹; ¹SCIEX, Redwood city, CA; ²Janssen, Spring House, PA
- WP 036 **Efficient and sensitive peptide mapping approach by µPAC columns with ultralow sample loading;** Yuan Lin¹; Xuefei Sun¹; Jeff Op De Beeck²; ¹Shanhua Lin¹; ¹Thermo Fisher Scientific, Sunnyvale, CA; ²Thermo Fisher Scientific, Ghent, Belgium
- WP 037 **Utilizing HRAM Orbitrap MS to Quantify Therapeutic Monoclonal Antibodies in Human Serum for Clinical Research;** Yvonne Ehwang Song¹; Stephanie N. Samra¹; Kerry Hassell¹; Julia Poncher¹; Bradley Hart¹; ¹Thermo Fisher Scientific, San Jose, CA

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- WP 038 **An ultra-sensitive and robust assay for an antibody-drug conjugate payload (paclitaxel) in human plasma using SLE-UPLC-MS/MS;** Andy (hongfang) Xue¹; Emily Williamson¹; Daniel Skrocki¹; Min Meng²; Aihua Liu¹; ¹Alliance Pharma, Malvern, PA; ²Chongqing Denali Medpharma Co.,Ltd, Chongqing, China
- WP 039 **LC-MS Characterization of Multi-Specific Antibodies;** Jeremy Wolff¹; Vera B. Ivleva¹; Yile Li¹; Melissa Resto¹; Jason G. Gall¹; Q. Paula Lei¹; ¹NIH, Gaithersburg, MD
- WP 040 **Conformation of Native Antibody-Drug Conjugate Charge Variants Revealed by Microchip Capillary Electrophoresis Coupled with Trapped Ion Mobility;** Eli J Larson¹; Adi M Kulkarni²; Jake A Melby³; Matthew Fischer³; Zhan Gao⁴; Kevin M. Buck³; Melissa R. Pergande⁴; Yanlong Zhu⁵; Guillaume Tremintin⁶; Kate Yu²; Ying Ge^{3,4,5}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²908 Devices, Inc., Boston, MA; ³Department of Chemistry, University of Wisconsin - Madison, Madison, WI; ⁴Department of Cell and Regenerative Biology, University of Wisconsin - Madison, Madison, WI; ⁵Human Proteomics Program, University of Wisconsin - Madison, Madison, WI; ⁶Bruker Daltonics, San Jose, CA
- WP 041 **Rapid identification of conjugation sites in antibody drug conjugates using Microchip Capillary Electrophoresis Coupled with Mass Spectrometry;** Yue Ju¹; Adi M Kulkarni²; Hampus Engstroem²; Erin Redman²; Kate Yu²; Guillaume Tremintin¹; ¹Bruker Daltonics, San Jose, CA; ²908 Devices, Inc., Boston, MA
- WP 042 **Analyses of chemical modifications in therapeutic antibodies by high resolution multi-turn TOF-MS system;** Yusuke Tateishi¹; Hiroyuki Miura¹; Hiroko Morinaga¹; Koichi Kimura¹; Tetsuo Iida¹; Junna Nakazono¹; Masaru Nishiguchi¹; Osamu Furuhashi¹; Daisuke Okumura¹; Yuki Yamaguchi²; Susumu Uchiyama²; ¹SHIMADZU Corporation, Kyoto, Japan; ²Osaka University, Suita, Osaka, Japan
- WP 043 **Improved intact antibody characterization with a new ion source design;** Kilian Mayr¹; Daniel Jajcevic¹; Lauren Stempf¹; Christian Albers²; Dodge Baluya³; José Bonfiglio¹; Rebekka Kroiher¹; Annette Vogt¹; ¹Roche Diagnostics GmbH, Penzberg, Germany; ²Bruker Daltonik GmbH, Bremen, Germany; ³Bruker Scientific, San Jose, CA
- WP 044 **Implementation of Multi-Attribute Method in the context of continuous biopharmaceutical manufacturing: from clone selection to analytical support in GxP runs;** Mélanie Jakobczyk; Merck KGaA, Darmstadt, Germany, Corsier-Sur-Vevey, Switzerland
- WP 045 **Investigation of drug-to-antibody ratio for FORCE oligonucleotide conjugates using Microchip CE-MS;** Benjamin F. Vieira¹; Aditya Kulkarni²; Kate Yu²; Peiyi Shen¹; Pei-Ni Tsai¹; Timothy Weeden¹; ¹Dyne Therapeutics, Inc., Waltham, MA; ²908 Devices, Inc., Boston, MA
- WP 046 **Structural Characterization of Biopharmaceutical Proteins using Ion-Mobility and Collision Induced Unfolding;** Kristine F Parson¹; Margo Wilson¹; Hunter Walker¹; Greg Adams¹; ¹FUJIFILM Diosynth Biotechnologies USA, Morrisville, NC
- WP 047 **Sensitive bioanalysis of galactosylsphingosine (GalSPH) and glucosylsphingosine (GluSPH) in cerebral spinal fluid;** Kean Woodmansey¹; Jack Steed¹; Jessica Smith¹; Freddy Oostebing²; Jianru Stahl-Zeng³; ¹SCIEX, Macclesfield, United Kingdom; ²Ardena Bioanalysis, Assen, Netherlands; ³SCIEX, Darmstadt, Germany
- WP 048 **5-Lipoxygenase Clinical Biomarker Method Development – Overcoming Selectivity, Stability, and Reagent Resourcing Challenges;** Liu Yang¹; John Meissen¹; Elske Franssen²; Anton I. Rosenbaum¹; ¹Integrated Bioanalysis, Clinical Pharmacology & Safety Sciences R&D, AstraZeneca, South San Francisco, CA; ²Translational Science and Experimental Medicine, Respiratory & Immunology, BioPharmaceuticals R&D, AstraZeneca, Cambridge, United Kingdom
- WP 049 **Improvement in quantitation targeting 270 human plasma proteins by MRM/MS with stable-isotope-labelled internal standards when automated nanoparticle fractionation i;** Claudia Gaither^{1,2}; Robert Popp¹; Aaron S. Gajadhar³; Paul Pease³; Lucy Williamson⁴; Asim Siddiqui⁴; Christoph H. Borchers^{5,6,7,8}; ¹MRM Proteomics Inc., Montréal, QC; ²Département de Biomédecine Vétérinaire, Faculté de Médecine Vétérinaire, Université de Montréal, Saint-Hyacinthe, QC; ³Seer Inc., Redwood City, CA; ⁴Seer, Inc., Redwood City, CA; ⁵Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ⁶Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ⁷Division of Experimental Medicine, McGill University, Montreal, QC; ⁸Department of Pathology, McGill University, Montreal, QC
- WP 050 **Quantitative Glycoproteomic Analysis of High-Density Lipoproteins in Alzheimer's Disease using LC-MS/MS;** Armin Oloumi¹; Brian Hong¹; Yasmine Bouchibti¹; Michael Russelle S. Alvarez¹; Angela M. Zivkovic¹; Carlito B. Lebrilla¹; ¹UC Davis, Davis, CA
- WP 051 **A stringently controlled, LC-MS-based strategy to procure interstitial fluid with minimal intra-cellular contamination from tissues;** Min Ma^{1,2}; Shihan Huo¹; Shichen Shen¹; Ming Zhang¹; Jun Qu^{1,2}; ¹University at Buffalo, Buffalo, NY; ²Roswell Park Comprehensive Cancer Center, Buffalo, NY
- WP 052 **Advancements in supercritical fluid chromatography-mass spectrometry expand the horizons for the analysis of smaller molecules in complex samples;** Kumari Ubhayasekera¹; Jonas Bergquist²; ¹Uppsala University, Uppsala, Sweden; ²Uppsala University, Uppsala, Sweden
- WP 053 **LC-MS/MS quantification of pTau217 using sepcific immunocapture in the context of Alzheimer's disease;** Florine Leipp^{1,2}; Sylvain Lehmann²; Christophe Hirtz²; Jerome Vialaret²; ¹Shimadzu France, Noisiel, France; ²IRMB-PPC, INM, CHU Montpellier, INSERM CNRS, Montpellier, France
- WP 054 **Proteomic analysis of amniotic fluid from Myelomeningocele fetuses unveils specific upregulation of nervous system development key proteins;** Lucie Guilbaud^{1,2}; Kevin Roge³; Andree Schmid^{4,5}; Cerina Chhuon⁶; Stefan Breimann^{4,5}; Joanna Lipecka⁷; Sophie Dreux⁸; Mueller Stefan^{4,5}; Michel Zerah⁹; Jerome Larghero⁹; Jean-Marie Jouannic¹; Stefan Lichtenthaler^{4,5}; Chiara Guerrero⁴; ¹Sorbonne University, Department of Fetal Medicine, AP-HP, Armand Trousseau Hospital, DMU ORIGYNE, National Reference Center for Rare Disease: Vertebral and Spinal Cord Anomalies (MAVEM Center), Paris, France; ²Paris University, Stem Cell Biotechnologies Unit, INSERM 976, CIC-BT CBT501, AP-HP, Saint-Louis Hospital, Paris, France; ³Proteomics Platform Necker, Paris, France; ⁴German Center for Neurodegenerative Diseases (DZNE), Munich, Germany; ⁵Neuroproteomics, School of Medicine, Klinikum Rechts der Isar, Technische Universität München, Munich, Germany; ⁶Proteomics Platform Necker, Paris, France; ⁷Proteomics Platform Necker, Paris, France; ⁸Paris University, Biochemistry-Hormonology, AP-HP, Robert Debré Hospital, Paris, France; ⁹Paris University, Department of Pediatric Neurosurgery, AP-HP, Hôpital Necker-Enfants Malades, Paris University, Paris, France
- WP 055 **The mucin selective protease StcE improves proteomic profiling of mucin containing human airway samples enhancing biomarker discovery in respiratory disease;** Lisa H. Cazares¹; Raghothama Chaerkady¹; Chiung-Yun Chang¹; Abby J. Chiang¹; Helen Killick²; Jessica Holmén Larsson²; Ian Christopher Scott²; Sonja Hess¹;

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- ¹AstraZeneca R&D, Gaithersburg, Maryland; ²AstraZeneca, Cambridge, United Kingdom
- WP 056 **Absolute quantification of plasma biomarkers to validate the first blood-based diagnosis of the silent phase of Alzheimer's Disease**; Antoine Berthemy¹; Maud Heuillet¹; Aude Dupuy-Gayral¹; Eloi Haudebourg¹; Catherine Pech¹; Benoît Souchet²; Alkéos Michail²; Baptiste Billoir²; Jérôme Braudeau²; François Autelitano¹; ¹EVOTEC, Toulouse, France; ²AgenT, Paris, France
- WP 057 **Development and evaluation of a rapid LC-MS/MS quantitation method for the measurement of reactive aldehydes in biological samples**; Yuanyuan Ji¹; Yulemni Morel¹; Anh Tran¹; Jace W. Jones¹; ¹University of Maryland, School of Pharmacy, Baltimore, MD
- WP 058 **Development of biomarkers for the delayed effects of acute radiation exposure: evaluation of diagnostic, predictive, and pharmacodynamic utility**; Swarnima Pandey¹; Nageswara Pilli¹; William Temple Andrews¹; Ludovic Muller¹; Maureen Kane¹; ¹University of Maryland School of Pharmacy, Baltimore, MD
- WP 059 **Enhanced LC-MS Analysis of Volatile Organic Compound Metabolites in Wastewater**; David Hoetker¹; Zhengzhi Xie¹; Pawel Lorkiewicz¹; Ted Smith²; Sanjay Srivastava³; ¹Christina Lee Brown Envirome Institute, University of Louisville, Louisville, KY; ²Center for Healthy Air Water Soil, University of Louisville, Louisville, KY; ³Superfund Research Center, University of Louisville, Louisville, KY
- WP 060 **Herding PCATs: Development of a Robust, High-Throughput Method for Quantification of Native Plasma Catecholamines by LC-MS/MS**; Stacy Dee¹; Christopher M. Shuford¹; Russell P Grant¹; ¹LabCorp, Burlington, NC
- WP 061 **Highly sensitive analysis using EVOSEP-LC/MS assay for targeted PD-L1 and PD1 expression level for predicting response to immune checkpoint inhibitors**; Shane Karnik¹; Matthew Hartle¹; Melodie Boute²; Richard Ruez²; Corinne Ramos²; ¹Pyxant Labs, Inc., Colorado Springs, CO; ²ImaBiotech, Loos, France
- WP 062 **Isotyping Anti-Drug Antibodies using LC-MS/MS QTOF quantification of SIL peptides**; Cristian I. Ruse¹; Ashish Vaswani¹; Carl Luongo¹; Hannah Zhang¹; Srujan Gandham¹; Matthew Digby¹; Jason Delcarpini¹; Darshana Jani¹; Ling Morgan¹; Serenus Hua¹; ¹Moderna Therapeutics, Cambridge, MA
- WP 064 **Online Enrichment of Low-Abundance Protein Biomarkers for Targeted LC-MS**; Nathaniel B. Axtell¹; Thy Truong¹; Alex Butters¹; Jeffrey R. Whiteaker²; Lei Zhao²; Amanda G. Paulovich²; Ryan T. Kelly¹; ¹BYU, Provo, UT; ²Fred Hutchinson Cancer Center, Seattle, WA
- WP 065 **Proteomic Profiling of Irradiation-Induced Skin Fibrosis and its modulation by Low Molecular Weight Fucoidan**; Pang-Hung Hsu; ¹National Taiwan Ocean University, Keelung, Taiwan
- WP 066 **Quantitative Analysis of Protein Ions Based in Isotopic Pattern Distortions**; Snehin R Momin¹; Touradj Solouki¹; ¹Baylor University, Waco, TX
- WP 067 **The Detection and Quantitation of Stercobilin in Autism Model Fecal Extracts Using LC-MS**; Erin R. Tiede¹; Emily R. Sekera²; Troy D. Wood¹; ¹University at Buffalo, Buffalo, NY; ²The Ohio State University, Columbus, OH
- WP 068 **timsTOF HT improves protein identification and quantitative reproducibility for deep unbiased plasma protein biomarker discovery**; Dijana Vitko¹; Wan-Fang Chou¹; Mark Marispini¹; Sai Ramaswamy¹; Sara Nouri Golmaei¹; Yuntao Hu¹; Joon Yong-Lee¹; Megan Mora¹; Jessica Chan¹; Guillermo Flores-Campuzano²; John Blume¹; Chinmay Belthangady¹; Manway Liu¹; Philip Ma¹; Bruce Wilcox¹; ¹PrognomiQ, San Mateo, CA; ²Switch Therapeutics Inc., San Francisco, CA
- WP 069 **Using a Specific Antibody for the Immunocapture LC-MS/MS Assay of the Biomarker, Troponin Fast (TNNI2)**; Shane Needham¹; Mitch Johnson¹; Colt Cookson¹; Joe Flynn¹; Ron Bowsher²; Derrick Johnson²; Sanofar Jainul Abdeen²; Molly Madden³; Ben Barthele³; ¹Velocity Labs, LLC, Peoria, IL; ²B2S Life Sciences, Franklin, IN; ³Edgewise Therapeutics, Boulder, CO
- WP 071 **Mapping of the Human Cell Metabolome Identifies Novel Cancer Therapeutic Targets in MYC-amplified Group 3 Medulloblastoma**; William D Gwynne¹; Yujin Suk²; Jeremy K Chan¹; Stefan Custers²; Cunjie Zhang¹; Andrew T Quaile¹; Chitra Venugopal²; Sheila K. Singh²; Rafael Montenegro-Burke¹; ¹Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; ²Center for Discovery in Cancer Research, McMaster University, Hamilton, ON
- WP 072 **The Identification of the HLA Class I Immopeptidome of Malignant Peripheral Nerve Sheath Tumors via Mass Spectrometry**; Kyle A Richards¹; Suzanne Coleman¹; Jessica Liebau¹; Mitchell Hruska¹; Tyler Jubenville^{1,2}; Reid Wagner²; Subina Mehta³; David A Largaespada^{1,2}; Timothy J Griffin³; ¹Masonic Cancer Center, Department of Pediatrics, University of Minnesota, Minneapolis, MN; ²Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN; ³Biochemistry, Mol. Biology, and Biophysics, University of Minnesota, Minneapolis, MN
- WP 073 **Detecting impending infections in immunocompromised cancer patients**; Sara Violante¹; Ruben J. F. Ramos¹; Hannah Lees¹; Emma E. Rennie²; James S. Pyke²; Andrew D. McEachran²; Mark Sartain²; Justin R. Cross¹; ¹Memorial Sloan Kettering Cancer Center, New York, NY; ²Agilent Technologies, Santa Clara, CA
- WP 074 **Multimetric approach to elucidate the role of endoplasmic reticulum-mitochondria contact sites in tumor metabolic rewiring**; Brandon Chen¹; Pietro Morlacchi²; Costas Lyssiotis¹; Yatrik Shah¹; ¹University of Michigan-Ann Arbor, Ann Arbor, MI; ²Agilent Technologies, Lexington, MA
- WP 075 **Targeted proteomics for discovery of novel biomarkers in human plasma for early breast cancer diagnosis**; Margret Thorsteinsdottir¹; Kristrun Yr Holm¹; Kari Annarsson¹; Finnur Eiriksson¹; Sigridur Klara Bodvarsdottir²; Yassene Mohammed³; Christoph H. Borchers⁴; ¹Faculty of Pharmaceutical Sciences, University of Iceland, Reykjavik, Iceland; ²BioMedical Center, University of Iceland, Reykjavik, Iceland; ³Leiden University Medical Center, Leiden, Netherlands; ⁴Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC
- WP 076 **Mass spectrometry-based proteomic profiling of CB-5083 resistant colon cancer cells**; Ting-Yu Wang¹; Feng Wang¹; Shan Li¹; Chai Foong Lai¹; Tsui-Fen Chou¹; ¹California Institute of Technology, Pasadena, CA
- WP 077 **Quantitative proteomic analysis of MCF10A cells with PTEN knockout reveals the regulation of Epha2 expression by PTEN**; Qiong Wang¹; Hongming Song¹; Li Wang¹; Santosh Renuse²; Kiran Mangalaparthy¹; Akhilesh Pandey¹; Xinyan Wu¹; ¹Mayo Clinic, Rochester, MN; ²Thermo Fisher Scientific, San Jose, CA
- WP 078 **Identification of Cholesterol and Cholesterol Derivatives in Prostate Cancer Cell Lines using Desorption Electrospray Ionization Mass Spectrometry**; Sarah Bench¹; Manoj Kumar¹; Daniel E Frigo²; Thomas L Pulliam²; Livia S. Eberlin¹; ¹Department of Surgery, Baylor College of Medicine, Houston, Texas; ²Department of Cancer Systems Imaging, The University of Texas MD Anderson Cancer Center, Houston, Texas
- WP 079 **Computational discovery of protein isoforms associated with drug response in breast cancer**; Lindsey Olsen^{1,2}; Yongchao Dou^{1,2}; Bing Zhang^{1,2}; ¹Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; ²Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX
- WP 080 **Comparative Proteomics studies of mono and co-cultured drug-resistant and -sensitive cancer cells**

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- reveal potential interaction targets; Zongkai Peng¹; Zhibo Yang¹; Ahsan Nagib^{1,2}; ¹University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; ²Mass Spectrometry, Proteomics and Metabolomics Core Facility, Stephenson Life Sciences Research Center, The University of Oklahoma, Norman, OK
- WP 081 **Integrated Omics approaches to understand Pituitary Adenomas disease biology;** Arghya Banerjee¹; Sanjeeva Srivastava¹; ¹IIT Bombay, Mumbai, India
- WP 082 **Role of MGAT3 and “Bisecting GlcNAc” N-glycans in TGF- β 1 induced epithelial-mesenchymal transition (EMT) of lung adenocarcinoma;** Wei Ge; Soochow University, Suzhou, China
- WP 083 **Using lipidomics analysis to determine the metabolic impact of PIKfyve inhibition in Pancreatic Ductal Adenocarcinoma;** Caleb Cheng¹; Pietro Morlacchi²; Li Zhang³; Pete Sajjakulnkit⁴; Jasmine Wisniewski⁵; Bailey Jackson⁵; Yuanyuan Qiao⁶; Costas Lyssiotis⁷; Arul M Chinnaiyan⁶; ¹Graduate Program in Cell and Molecular Biology, University of Michigan, Ann Arbor, Michigan; ²Agilent Technologies, Lexington, MA; ³School of Medicine, University of Michigan, Ann Arbor, Michigan; ⁴Doctoral Program In Cancer Biology, University of Michigan, Ann Arbor, Michigan; ⁵College of LSA, University of Michigan, Ann Arbor, Michigan; ⁶Michigan Center for Translational Pathology, Department of Pathology, University of Michigan, Ann Arbor, Michigan; ⁷Department of Molecular and Integrated Physiology, Department of Internal Medicine, University of Michigan, Ann Arbor, Michigan
- WP 084 **Initial Results from Mass Spectrometry Imaging Characterization of Liver Tumor Development in the Oncopig Model;** Danielle L Stolley¹; Maria Sophia Stenkamp¹; Natalie Fowlkes¹; Erin H Seeley²; Erik Cressman¹; ¹MD Anderson Cancer Center, Houston, TX; ²University of Texas at Austin, Austin, TX
- WP 085 **Top down proteomics reveals Histone H2A C-terminal truncations as potential modulators of DNA damage and cell proliferation in cancer;** Faith Joseph¹; Nicolas Leon Young^{2,3}; ¹baylor college of medicine, houston, TX; ²Verna & Marris McLean Department of Biochemistry & Molecular Biology, Baylor College of Medicine, Houston, TX; ³Department of Molecular and Cellular Biology, Baylor College of Medicine, Houston, TX
- WP 086 **Tumor intrinsic metabolic effects associated with inhibition of PARP7 in a lung cancer cellular model;** Jennifer R Molina¹; Pietro Morlacchi²; Jeffrey Song¹; Sonal Gera¹; ¹Ribon Therapeutics, Cambridge, Massachusetts; ²Agilent Technologies, Lexington, MA
- WP 087 **Integrated proteomics and metabolomics reveal an association between NFR2-mediated upregulation of KYNU and tumor immunosuppression and poor prognosis;** Ricardo A Leon Letelier¹; Ali Hussein Abdel Sater¹; Yihui Chen¹; Ranran Wu¹; Jennifer B Dennison¹; Soyoun Park¹; Ehsan Irajizad¹; Hiroyuki Katayama¹; Jody Vykoukal¹; Samir M Hanash¹; Edwin J Ostrin¹; Johannes Fahrman¹; ¹MD Anderson Cancer Center, Houston, TX
- WP 088 **Integrative Single-Organoid Proteomics in 3D Models of Ovarian Cancer Uncovers Remodeled Mitochondria-ER Contacts and Bioenergetics;** Krystal K Lum¹; Oscar Pundel²; William A Hofstadter¹; John Muroski¹; Benjamin G Neel²; Ileana M Cristea¹; ¹Princeton University, Princeton, NJ; ²NYU Langone Health, New York, NY
- WP 089 **Regulation of the FKBP10 transcriptional locus in lung metastasis;** Bryan Rivas¹; Alexander B. Saltzman¹; Doug Chan²; Anna Malovannaya¹; ¹Baylor College of Medicine, Houston, Texas; ²MD Anderson, Houston, TX
- WP 090 **Proteomics investigation of gliomas resected after 5-ALA fluorescence guided surgery reveals molecular heterogeneity driving differential fluorescence;** Saicharan Ghantasala¹; Amruth Bhat²; Aliasgar Moiyadi^{3,4}; Sridhar Epari^{3,4}; Sanjeeva Srivastava⁵; ¹Centre for Research in Nano Technology and Science, Indian Institute of Technology Bombay, Mumbai, India; ²Centre for BioSystems Science and Engineering, Indian Institute of Science, Bengaluru, India; ³Department of Neurosurgery, Tata Memorial Centre's – Advanced Centre for Treatment, Research and Education in Cancer, Navi Mumbai, India; ⁴Homi Bhabha National Institute, Mumbai, India; ⁵Department of Biosciences and Bioengineering, Indian Institute of Technology Bombay, Mumbai, India
- WP 091 **INFLUENCE OF MDR (MULTIDRUG RESISTANCE) AND CELL-CELL INTERACTIONS ON DRUG UPTAKE OF SPHEROIDS;** Amit Singh¹; Zongkai Peng¹; Zhibo Yang¹; Anthony Burgett²; ¹University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; ²The University of Oklahoma Health Sciences Center, College of Pharmacy, Oklahoma City, OK
- WP 092 **Assessing the Impact of Paclitaxel Absorption by 3D Breast Cancer Spheroids Using LC-MS/MS;** Ramisa Fariha¹; Zahra Ahmed¹; Jad Hamze¹; Emma Rothkopf¹; Oluwanifemi Okoh¹; Anubhav Tripathi¹; ¹Brown University, Providence, RI
- WP 093 **Identification of metabolic pathways driven by SMARCB1 deficiency in bladder cancer;** Chandra Sekhar Amara¹; Abu Hena Mostafa Kamal¹; Danthasinghe Waduge Badrajee Piyarathna¹; Arun Sreekumar¹; Msaouel Pavlos²; Nagireddy Putluri¹; ¹Baylor College of Medicine, Houston, Texas; ²MD Anderson, Houston, TX
- WP 094 **Identification of altered mitochondrial metabolism in bladder cancer disparity;** Karthik Reddy Kami Reddy¹; Junhyoung Park¹; Vasanta Putluri¹; Danthasinghe Waduge Badrajee Piyarathna¹; Martha K Terris²; Seth P Lerner¹; Yair Lotan³; Benny Abraham Kaiparettu¹; Nagireddy Putluri¹; ¹Baylor College of Medicine, Houston, TX; ²Augusta university, Augusta, Georgia; ³UT Southwestern Medical Center, Dallas, Texas
- WP 095 **LC-MS method to measure the D- and L-2-Hydroxyglutarate in Cerebrospinal Fluid;** Satwikreddy Putluri¹; Abu Hena Mostafa Kamal²; Leomar Y Ballester³; ¹University of Texas MD Anderson Cancer Center, Houston, TX; ²Baylor College of Medicine, Houston, Texas; ³MD Anderson, Houston, TX
- WP 096 **Application of the MasSpec Pen Technology for Molecular Identification of Human Sarcomas and Surgical Margin Evaluation;** Ashley E. Montgomery¹; Justin E. Bird²; Douglas Fletcher²; Sharon Landers³; Sintawat Wangsiricharoen⁴; Wei-Lien Wang⁴; Wendong Yu⁴; Livia S. Eberlin⁵; Keila E. Torres³; ¹Baylor College of Medicine, Department of Student Affairs, Houston, Texas; ²MD Anderson Cancer Center, Division of Surgery, Department of Orthopedics, Houston, Texas; ³MD Anderson Cancer Center, Division of Surgery, Department of Surgical Oncology, Houston, Texas; ⁴MD Anderson Cancer Center, Division of Pathology Lab-Medicine, Department of Pathology, Houston, Texas; ⁵Baylor College of Medicine, Division of Surgical Oncology, Michael E DeBakey Department of Surgery, Houston, Texas
- WP 097 **Probing the Biosynthetic Pathway of Heparan Sulfate Using Capillary Electrophoresis Zone Mass Spectrometry;** Jandi Kim¹; Neil G. Patel^{1,2}; Ryan Joseph Weiss^{1,2}; I. Jonathan Amster¹; ¹University of Georgia, Athens, GA; ²Complex Carbohydrate Research Center, Athens, GA
- WP 098 **Does The Chemistry of Glycosidic Bond Cleavage Vary?;** Joy Namachanja Malaba¹; Lauren Schultz¹; Lauren Davis¹; Dylan Carter²; Benjamin Bythell²; ¹Ohio University, Athens, OH; ²Ohio University, Athens, OH
- WP 099 **Combined Tandem Mass Spectrometry and Computational Chemistry for Structural Elucidation of Singly and Doubly Deprotonated Galacturonic Acids;** Ola Bataineh¹; Jordan Rabus¹; Rebecca Flinchbaugh¹; Dylan Carter¹; Lauren Davis¹; Benjamin Bythell¹; ¹Ohio University, Athens, OH

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- WP 100 **N-Glycan Quantitation and Characterization via HILIC-FLD-ESI/MS Using a Novel Fluorescence Free Radical Reagent**; Shane Finn¹; Rayan Murtada¹; Wilthon Gilles¹; Jinshan Gao¹; ¹Montclair State University, Montclair, NJ
- WP 101 **Mass Spectrometry-based High-throughput Profiling of Porcine Notochordal-Cell Matrix N-glycans Using Glycan Explorer™ Software**; Rupanjana Goswami¹; Kieran Joyce²; Büşra Günay²; Melanie Ng Tung Hing^{3,4}; Caitriona Walsh⁵; Tara Schmitz⁶; Marianna Tryfonidou⁷; Keita Ito⁶; Karthik Kolli¹; Abhay Pandit²; Radka Saldova^{2,3,4}; Arun Apte¹; ¹PREMIER Biosoft, San Francisco, CA; ²CURAM, SFI Research Centre for Medical Devices, National University of Ireland, Galway, Galway, Ireland; ³GlycoScience group, National Institute for Bioprocessing Research and Training (NIBRT), Dublin, Ireland; ⁴UCD School of Medicine, College of Health and Agricultural Science, University College Dublin, Dublin, Ireland; ⁵Contract Research group, National Institute for Bioprocessing Research and Training (NIBRT), Dublin, Ireland; ⁶Orthopaedic Biomechanics, Department of Biomedical Engineering, Eindhoven University of Technology, Eindhoven, Eindhoven, Netherlands; ⁷Department of Clinical Sciences, Faculty of Veterinary Medicine, Utrecht University, Utrecht, Netherlands
- WP 102 **Adduct Activity of Sheath Liquid CE-MS interface Depends on the Sheath Liquid Content for Glycosaminoglycans**; Jonathan Choi¹; I. Jonathan Amster¹; Jandi Kim¹; ¹University of Georgia, Athens, GA
- WP 103 **Characterizing degradation products from Bacteroides thetaiotaomicron to understand bacterial dextran utilization in the gut**; Neil Gregory Rumachik¹; Tian Tian¹; Hannah Gibson²; David Bolam²; Yan Liu¹; Fiona Cuskin²; ¹Thermo Fisher Scientific, Sunnyvale, CA; ²Newcastle University, Newcastle upon Tyne, United Kingdom
- WP 104 **Analysis of Chondroitin Sulfate Oligosaccharides in cartilage with mucopolysaccharidosis VII using Capillary Zone Electrophoresis–Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Elijah T Roberts¹; Jandi Kim¹; Stephanie Archer-Haartman^{1,2}; Lachlan James Smith³; Jonathan Amster¹; Zhirui Jiang⁴; Yian Khai Lau⁵; Margaret Casal^{3,5}; ¹University of Georgia, Athens, GA; ²Complex Carbohydrate Research Center, Athens, GA; ³University of Pennsylvania, Philadelphia, PA; ⁴Forsyth Institute, Cambridge, Massachusetts; ⁵University of Pennsylvania School of Veterinary Medicine, Philadelphia, Pennsylvania
- WP 105 **Isomeric Separation of Permethylated Glycans using LC-FAIMS-MS/MS**; Md Abdul Hakim¹; Akeem Adeyemi Sanni¹; Waziha Purba¹; Oluwatosin Daramola¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- WP 106 **Isomeric separation of native N-glycans using nano ZIC-HILIC column**; Oluwatosin E Daramola¹; Cristian D Gutierrez-Reyes¹; Judith Nwaiwu¹; Mojibola Fowowe¹; Sherifdeen Onigbinde¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- WP 107 **HCD, ETD, and EThcD Fragmentation Spectra of Co2+-Adducted Human Milk Oligosaccharides Distinguish Linkage Isomers**; Sebastian N Alberti¹; Darren Gass¹; Elyssia S. Gallagher¹; ¹Baylor University, Waco, TX
- WP 108 **Comprehensive Characterization of Functional Polysaccharides derived from Marine Algae**; Dae Sik Cho^{1,2}; Sol Kim^{1,2}; Hong Ju Kim^{1,2}; Nari Seo^{1,2}; Hyun Joo An^{1,2}; ¹Graduate School of Analytical Science and Technology, Chungnam National University, South Korea; ²Asia-Pacific Glycomics Reference Site, Daejeon, South Korea
- WP 109 **Mass spectrometry-based characterization of native and aging-modified polysaccharides for natural gums identification in complex formulations**; Marie Yammine^{1,2}; Hanane Termoul¹; Stéphanie Flament¹; Fabrice Bray¹; Christian Rolando^{1,3}; ¹UAR CNRS 3290 - MSAP, Villeneuve d'Ascq, France; ²Lesaffre International - R&D analytical department, Marquette-Lez-Lille, France; ³Shrieking Sixties - 1-3 Allée Lavoisier, Villeneuve d'Ascq, France
- WP 110 **Structural and compositional characterization of dissolved hemicellulose with 12-T ESIF-ICR in positive and negative ion modes**; Mikko Nikunen¹; Timo Kekäläinen¹; Janne Jänis¹; ¹University of Eastern Finland, Department of Chemistry, Joensuu, Finland
- WP 111 **Sensitive Analysis and Differentiation of Oligosaccharides Isomers by Direct Infusion Mass Spectrometry**; Enoch Amoah¹; Abraham Kwame Badu-Tawiah²; ¹The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; ²The Ohio State University, Columbus, OH
- WP 112 **Developing Novel capillary electrophoresis tandem mass spectrometry strategies for the characterization of complex mixture Heparan sulfates**; Yiqing Zhang¹; Jonathan Amster²; ¹University of Georgia, Department of Chemistry, Athens, GA; ²University of Georgia, Athens, GA
- WP 113 **Optimization of PRM-LCMS/MS for Glycosaminoglycan Disaccharide Profiling in C. Elegans**; Lauren Heidenreich¹; Franklin E. Leach III¹; ¹University of Georgia, Athens, GA
- WP 114 **Quantitation of glycosaminoglycans expression in cancer cells by 2-aminoacridone-labeled disaccharides with LC-MS/MS analysis**; Fu-An Li¹; Yu-Shing Cheng¹; ¹Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan
- WP 115 **A Novel LC-MS/MS Approach for Identification and Quantification for Hexosamine-Phosphates and Differentiate GlmS Regulation Between Staphylococcus aureus and Enterococcus faecium**; Nitish R. Mishra¹; William G. Gutheil¹; ¹University of Missouri-Kansas City, Kansas City, MO
- WP 116 **A window of opportunity: optimising diaPASEF approaches for liquid biopsy proteomics for a large-scale clinical cohort**; Samantha J Emery-Corbin^{1,2}; Megan Penno^{3,4}; Jumana M Yousef^{1,2}; Vineet Vaibhav^{1,2}; Helena Oakley³; Jennifer J Couper³; Leonard C Harrison^{2,4}; John M Wentworth^{2,4}; Toby Dite^{1,2}; Andrew I Webb^{2,5}; Laura F Dagley^{1,2}; ¹Advanced Technology and Biology Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Melbourne, Australia; ²Department of Medical Biology, University of Melbourne, Parkville, Melbourne, Australia; ³Faculty of Faculty Health and Medical Sciences, The University of Adelaide, Adelaide, Australia; ⁴Population Health Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Melbourne, Australia; ⁵Colonial Foundation Healthy Ageing Centre, Walter and Eliza Hall Institute of Medical Research, Parkville, Melbourne, Australia
- WP 117 **Fast multi-shot acquisition of comprehensive proteomes by DIA using narrow isolation windows on a novel high-resolution accurate mass LC/MS platform**; Ulises Hernandez Guzman¹; Ana Martinez Del Val¹; Zilu Ye¹; Florian Harking¹; Tabiwan N. Arrey²; Anna Pashkova²; Hamish Stewart²; Yue Xuan²; Nicolaie Eugen Damoc²; Jesper V. Olsen¹; ¹Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- WP 118 **Robust, Precise and Deep Proteome Profiling Using a Small Mass Range and Narrow Window Data-Independent-Acquisition Scheme**; Klemens Fröhlich^{1,2}; Christian Schori^{1,2}; Regula Furrer²; Alexander Schmidt^{1,2}; ¹Proteomics Core Facility, University of Basel, Basel, Switzerland; ²Biozentrum, University of Basel, Basel, Switzerland
- WP 119 **midia-PASEF maximizes information content in data-independent acquisition proteomics and uses machine learning based-deconvolution to generate DDA quality spectra**; Ute Distler¹; Mateusz Krzysztof Łacki¹; Michał

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- Piotr Startek¹; David Teschner²; Sven Brehmer³; Jens Decker³; Thilo Schild¹; Jonathan Krieger⁴; Florian Krohs³; Oliver Raether³; Andreas Hildebrandt²; Stefan Tenzer^{1,5}; ¹Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany; ²Institute for Informatics, Johannes-Gutenberg University Mainz, Mainz, Germany; ³Bruker Daltonics GmbH & Co.KG, Bremen, Germany; ⁴Bruker Ltd, Milton, ON; ⁵Helmholtz Institute for Translational Oncology (HI-TRON), Mainz, Germany
- WP 120 **Benchmarking commonly used software suites and analysis workflows for DIA proteomics and phosphoproteomics**; Ronghui Lou¹; Ye Cao²; Shanshan Li¹; Yaoyang Zhang²; Wenqing Shui¹; ¹ShanghaiTech University, Shanghai, China; ²Chinese Academy of Sciences, Shanghai, China
- WP 121 **Cross-lab Evaluation of Quality Control for Large-scale Data-Independent Acquisition-based quantitative proteomics**; Gaohuan Gao¹; He Wang¹; Yantao Li²; Zhongxiang Ni²; Yi Zhu¹; Tianan Guo¹; ¹Westlake University, Hangzhou, China; ²WestLake Omics Biotechnology Co., Ltd, Hangzhou, China
- WP 122 **The synchro-PASEF scan mode on a TIMS-q-TOF mass spectrometer for DDA-like specificity from DIA data**; Patricia Skowronek¹; Georg Wallmann¹; Maria Wahle¹; Ericka C. M. Itang¹; Polina Koval¹; Marvin Thielert¹; Florian Krohs²; Markus Lubeck²; Sander Willems³; Oliver Raether²; Matthias Mann^{1,4}; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Bruker Daltonics GmbH & Co.KG, Bremen, Germany; ³Bruker Belgium nv, Kontich, Belgium; ⁴Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark
- WP 123 **Multiplexed data-independent acquisition (DIA) using a novel high-resolution accurate mass spectrometer**; Sophia Steigerwald¹; Wen-Feng Zeng¹; Maximilian T. Strauss²; Marvin Thielert¹; Ulises H. Guzmán²; Nicolaie Eugen Damoc³; Stevan Horning³; Jesper V. Olsen²; Matthias Mann^{1,2}; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, København, Denmark; ³Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- WP 124 **Single-Shot deep DIA LCMS workflow for near-full proteome coverage**; Robert Van Ling¹; Amirmansoor Hakimi²; Santosh Renuse²; Paul Jacobs³; Jeff Op De Beeck³; ¹Thermo Fisher Scientific, Breda, Netherlands; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific - Belgium, Ghent, Belgium
- WP 125 **BiblioPlasma: A gateway for dia-PASEF analysis with a library assembled from 4500 depleted plasma runs**; Jonathan R Krieger¹; Patrick Von Zalm²; Arthur Viode²; Hanno Steen^{2,3}; Judith Steen⁴; ¹Bruker Ltd., Milton, ON; ²Department of Pathology, Boston Children's Hospital, Harvard Medical School, Boston, MA; ³Neurobiology Program and Precision Vaccines Program, Boston Children's Hospital, Boston, MA; ⁴Neurobiology Program, Boston Children's Hospital, Harvard Medical School, Boston, MA
- WP 126 **Rapid and integrated proteome and lipidome analysis of mouse livers using Multi-Omic Single-Shot Technology and Data Independent Acquisition**; Margaret Lea Robinson¹; Yuchen He²; Evgenia Shishkova²; Katherine A Overmyer^{2,3}; Joshua J. Coon^{2,3}; ¹University of Wisconsin, Madison, Madison, WI; ²University of Wisconsin-Madison, Madison, WI; ³Morgridge Institute for Research, Madison, WI
- WP 127 **Deciphering the molecular pathway driving cell competition using DIA label-free mass spectrometry**; Suniya Khatun¹; Riccardo Zenezini Chiozzi^{1,2}; Manasi Kelker³; Guillaume Charras^{3,4,5}; Alan Lowe^{1,3,4,6}; Konstantinos Thalassinou^{1,2,7}; ¹Department of Structural and Molecular Biology - UCL, London, United Kingdom; ²Mass Spectrometry Science Technology Platform - UCL, London, United Kingdom; ³London Centre for Nanotechnology - UCL, London, United Kingdom; ⁴Institute for the Physics of Living Systems - UCL, London, United Kingdom; ⁵Department of Cell and Developmental Biology - UCL, London, United Kingdom; ⁶The Alan Turing Institute, London, United Kingdom; ⁷Institute of Structural and Molecular Biology - Birkbeck College, London, United Kingdom
- WP 128 **Data-independent acquisition leverages untargeted proteomics in microbes to quantify both engineered and endogenous protein abundances**; John Muroski¹; Gabriel Navarro¹; Mona Elbadawi¹; ¹Amyris, Emeryville
- WP 129 **Optimizing dia-PASEF isolation window schemes for proteomics measurements on a timsTOF instrument**; Markus Lubeck¹; Stephanie Kaspar-Schoenefeld¹; Christoph Krisp¹; Andreas Schmidt¹; Florian Busch¹; Eduardo Carrascosa¹; Oliver Raether¹; Gary Kruppa²; ¹Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ²Bruker S.R.O., Brno, Czech Republic
- WP 130 **Integrating permethylation and Zeno SWATH method to characterize nucleic acid modifications**; Yixuan (axe) Xie¹; Ye Chen¹; Francisca N De Luna Vitorino¹; Zongtao Lin¹; Xingyu Liu¹; Emily Zahn¹; Arabella Garcia¹; Benjamin A. Garcia¹; ¹Washington University in St.Louis, St.Louis, MO
- WP 131 **DIA makes the difference:DIA-CF-MS outperforms DDA-CF-MS for predicting protein interactions in a non-model organism**; Mopelola O. Akinlaja¹; Brenna H. Hay¹; Teesha C. Baker¹; Aicha A. Houfani¹; Greg R. Stacey¹; Leonard J. Foster¹; ¹University of British Columbia, Vancouver, BC
- WP 132 **Data-Independent Analysis of Human Eye Lens Proteome Reveals New Sites of Aspartic Acid Isomerization**; Evan E Hubbard¹; Yana Lyon^{2,3}; Ryan R. Julian¹; ¹University of California, Riverside, Riverside, CA; ²Inhibrx Inc., La Jolla, 92037; ³University of California Riverside, Riverside, CA
- WP 133 **Achieving robust quantitative analysis of proteomes using Vacuum insulated probe heated electrospray ionization (VIP-HESI) coupled with microflow chromatography and timsTOF-Mass-Spectrometer**; Mukul K. Midha¹; Charu Kapil¹; Michal Maes¹; David H. Baxter¹; Seamus R. Morrone¹; Timothy J. Prokop¹; Robert L. Moritz¹; ¹Institute for Systems Biology, Seattle, WA
- WP 134 **Application of advanced targeted MS and long-read RNA-seq for proteogenomic discovery and expanded detection of alternative protein isoforms**; Saikat Bandyopadhyay¹; Erin D. Jeffery¹; Qing Yu²; Ben Jordan³; Gloria Sheynkman^{1,4,5,6}; ¹Department of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville, Virginia, USA, Charlottesville, VA; ²Department of Cell Biology, Harvard Medical School, Boston, MA, USA, Boston, MA; ³Cancer Genomics Research Laboratory, Frederick National Laboratory for Cancer Research, Frederick, MS USA, Frederick, MD; ⁴Department of Biochemistry and Molecular Genetics, University of Virginia, Charlottesville, VA, USA, Charlottesville, VA; ⁵Center for Public Health Genomics, University of Virginia, Charlottesville, VA, USA, Charlottesville, VA; ⁶UVA Comprehensive Cancer Center, University of Virginia, Charlottesville, VA, USA, Charlottesville, VA
- WP 135 **Optimization and evaluation of precursor isolation schemes in midiaPASEF acquisition mode**; Ute Distler¹; Mateusz Krzysztof Łacki¹; Michał Piotr Startek²; David Teschner³; Jonathan Krieger⁴; Florian Krohs⁵; Oliver Raether⁵; Stefan Tenzer¹; ¹Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany; ²Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; ³Institute for Informatics,

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- Johannes-Gutenberg University Mainz, Mainz, Germany; ⁴Bruker Ltd, Milton, ON L9T 6P4; ⁵Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- WP 136 **Doing More With Less: Addressing The MicroSampling Sensitivity Challenge in DMPK Studies Using Vacuum Jacketed Column UHPLC-cyclic Ion Mobility MS**; Robert Plumb¹; Andrew Lightner¹; Ian D Wilson²; Billy J Molloy³; Russell Mortishire-Smith³; ¹Waters, Milford, MA; ²Imperial College, London, London, United Kingdom; ³Waters Corporation, Wilmslow, United Kingdom
- WP 137 **Ultra-High Throughput Metabolic Stability Assay using Acoustic Ejection Mass Spectrometry**; Jacob Watson McCabe¹; Anuja Bhalkikar¹; Han Joo Lee¹; ¹SCIEX, Frammingham, MA
- WP 138 **Assessment of Chromatographic Performance in High-Throughput ADME Screening**; Carson Powell¹; John Janiszewski¹; Ross Wallace¹; ¹Loxo Oncology, Louisville, CO
- WP 139 **Improving the workflow of pharmacokinetic study of herbal medicines, Cudrania tricuspidata leaf extracts, using molecular networking**; Jeong In Seo^{1,2}; Hye Hyun Yoo¹; ¹Hanyang University, Ansan, South Korea; ²Brigham and Women's Hospital, Boston, MA
- WP 140 **Automated workflow to study microsomal clearance and analysis of metabolites using collision-induced dissociation and electron-activated dissociation MS/MS data**; Bahar Rizzi¹; Rahul Baghla²; Eshani Nandita²; ¹Sciex, Frammingham, MA; ²SCIEX, Redwood City, CA
- WP 141 **An efficient permeability screening flow using LC-MS/MS based PAMPA assay followed by MDCK assay of selected compounds**; Yongying Jiang¹; Phuong Nguyen¹; Quanyun Alan Xu¹; Qi Wu¹; Thomas Quill¹; ¹University of Texas MD Anderson Cancer Center, Houston, TX
- WP 142 **Metabolite profiling and characterization by ion mobility LC-timsTOF Pro PASEF**; Xuejun Peng¹; Surendar Tadi²; Beixi Wang¹; Erica Forsberg¹; ¹Bruker Daltonics Inc., San Jose, CA; ²Bruker Scientific, LLC, Billerica, MA
- WP 143 **Reducing Turnaround Time and Compound Consumption for ADME Screening with Echo® Liquid Handling and Automation Enabling High Capacity LC-MS/MS Assays**; Ashley A. Rehm¹; Birju Patel¹; Mitchell J. Martineau¹; Shantanu Roychowdhury¹; ¹Eurofins Panlabs, Saint Charles, MO
- WP 144 **Global profiling of AMG510 modified proteins identified tumor suppressor KEAP1 as an off-target**; Yini Wang¹; Bowen Zhong²; Caixia Xu²; Dongdong Zhan²; Yi Wang²; Jun Qin²; ¹National Center for Protein Sciences (The PHOENIX Center, Beijing), Beijing, China; ²National Center for Protein Sciences (The PHOENIX Center, Beijing), Beijing, China
- WP 145 **LC-MS metabolic profiling of a standardized extract of PACs from Vitis vinifera seeds in healthy volunteers and in-vitro supporting studies**; Giovanna Baron¹; Larissa Della Vedova¹; Francesca Gado¹; Laura Fumagalli¹; Marina Carini¹; Cristian Del Bo²; Paolo Morazzoni³; Giancarlo Aldini¹; ¹Department of Pharmaceutical Sciences (DISFARM), Università degli Studi di Milano, Milan, Italy; ²Department of Food, Environmental and Nutritional Sciences, Università degli Studi di Milano, Milan, Italy; ³Divisione Nutraceutica, Distillerie Umberto Bonollo S.p.A, Mestrino, Italy
- WP 146 **Determination of Bicalutamide in Human and Mouse serum using PerkinElmer QSign 420 LC-MS/MS system with Epic C18 column**; Sergey Shulga-Morskoy¹; Cole Stratman²; ¹Perkin Elmer Health Sciences Inc, Hopkinton, MA; ²Perkin Elmer, Shelton, CT
- WP 147 **Open Port Interface with Electromagnetic Mixing for an Affinity Selection MS System**; Thomas R. Covey¹; Chang Liu¹; Peter Kovarik¹; Jonathan Shrimp²; Nate Hoxie²; Michael Ronzetti²; Bolormaa Baljinnyam²; Colin Kelly²; John Janiszewski²; Meghav Verma²; Sam Michael²; Matthew Hall²; Anton Simeonov²; Richard Van Breemen³; Yuandan Liu⁴; Jianli Zhao⁴; Emmet Welch⁴; ¹SCIEX, Concord, ON; ²National Center For Advancing Translational Sciences, Rockville, MD; ³Oregon State University, Corvallis; ⁴Phenomenex, Torrance, CA
- WP 148 **Microtiter well based MS method scheduling for high-throughput mass spectrometry**; David Cox¹; Chang Liu¹; Bogdan Georgescu¹; ¹SCIEX, Concord, ON
- WP 149 **Investigating CYP Reaction Phenotyping using HEPATOPAC® for Low Turnover Compounds: Identifying Inhibitor for CYP2B6 and Describing Temporal CYP1A2 Activity Decline**; Mark Athanason¹; Sheri Smith¹; Bennett Ma¹; Karsten Menzel¹; ¹Pharmacokinetics, Merck & Co., Inc., West Point, Pennsylvania
- WP 150 **Quantitative Assessment of Membrane Transporters in Rat and Human Hepatocytes for Model Informed Drug Development**; Mariel R Mendoza¹; Mark Athanason¹; Michelle Robinson¹; Xiaoyan Chu¹; Jingjing Guo¹; Matthew Mazur¹; Weixun Wang¹; ¹Merck & Co., Inc., West Point, PA
- WP 151 **Mitragynine UPLC-MS/MS Method Development and Preclinical Pharmacokinetics**; China Ryu¹; Natalie R. Hagen¹; Junfeng Huang¹; Xin Xu¹; Amy Q. Wang¹; ¹National Center for Advancing Translational Sciences, National Institutes of Health, Rockville, MD
- WP 152 **Improved Performance of a Milli fluidic System for Drug Absorption Studies using ex vivo tissue and Mass Spectrometry**; Chloe E Spencer¹; Malcolm R. Clench¹; Vikki Carolan¹; Stephen Rumbelow²; ¹BMRC, Sheffield Hallam University, Sheffield, United Kingdom; ²CRODA Inc, New Castle, Delaware
- WP 153 **Metabolites of the Large Cyclic Peptide Antibiotic Cyclosporin A Characterized Using HPLC/ESI-Exact-Mass-MS/MS Data with MASSPEC Structure Elucidation Software**; Marshall M. Siegel¹; Gary E Walker¹; Serhiy Hnatyshyn²; ¹MS Mass Spec Consultants, Fair Lawn, NJ; ²BMS, Princeton, NJ
- WP 154 **Chemical derivatization coupled with 2D-LC-MS/MS enabling sensitive quantitation of SEP-383103 (a major metabolite of ulotaront) in Rat Plasma**; Yu-Luan Chen¹; Jingduan Chi²; Melissa Mofikoya²; Lei Shi¹; ¹Sunovion Pharmaceuticals Inc., Marlborough, MA; ²PPD, Middleton, WI
- WP 155 **Quantification of Sazetidine-A from Rat Brain and Plasma for the Treatment of Tinnitus**; Emily M Hubecky¹; Samantha A Olendorf²; Donald Caspary³; Lynne Ling³; Kevin R Tucker¹; ¹Southern Illinois University Edwardsville, Edwardsville, Illinois; ²Shimadzu, Columbia, MD; ³Southern Illinois University School of Medicine, Springfield, IL
- WP 156 **A Highly Sensitive 2D-LC/MS/MS Method for the Quantitation of Ethinyl Estradiol and Etonogestrel in Human Plasma**; Jingduan Chi¹; Melissa Mofikoya¹; Zhijing Huang¹; ¹PPD Inc, Madison, WI
- WP 157 **Analysis of apixaban, dabigatran and metabolites in human liquid specimens using vortex-assisted salt-enhanced liquid-liquid microextraction coupled with UHPLC-MS/MS**; Tzu-Yu Pan¹; Chia-Fang Wu^{1,2}; Ming-Tsang Wu^{3,4,5,6}; ¹Kaohsiung Medical University Research Center for Environmental Medicine, Kaohsiung city, Taiwan; ²International Master Program of Translational Medicine, National United University, Miaoli city, Taiwan; ³Kaohsiung Medical University Research Center for Environmental Medicine, Kaohsiung city, Taiwan; ⁴Ph.D. Program in Environmental and Occupational Medicine, College of Medicine, Kaohsiung Medical University, Kaohsiung city, Taiwan; ⁵Department of Public Health, College of Health Sciences, Kaohsiung Medical University, Kaohsiung city, Taiwan; ⁶Department of Family Medicine, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Kaohsiung city, Taiwan
- WP 158 **Determination of Ethyl Glucuronide in plasma by ATLAS-LEXT NHD combined with LC-MS/MS**; Chen

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- Jianli¹; Li Qiang²; Hao Hongyuan²; ¹Shimadzu (China) Co., Ltd., Wuhan, China; ²Shimadzu(China)Co.,LTd, Shanghai, China
- WP 159 **Structure elucidation of a macrocyclic GSH-adduct metabolite of Rilzabrutinib, a reversible covalent BTK inhibitor;** Cathy Muste¹; Shu-Yu Liao¹; Chungang Gu¹; ¹Biogen, Cambridge, MA
- WP 160 **Novel Application of LC-MS to Qualitatively Identify Underivatized Metoprolol Acid in Equine Plasma to Prove Metoprolol Administration;** Benjamin J Burris¹; Halie A Copley¹; Mark A Musetti¹; Deidre E Damon¹; Ryan M Farmer¹; Soobeng Tan¹; ¹Ohio Department of Agriculture, Reynoldsburg, OH
- WP 161 **Exploring the Applicability of Multi-Reflecting Time-of-Flight Mass Spectrometry for Expedited Biotransformation Studies;** Daniel J Weston¹; Emma Marsden-Edwards²; Martin Palmer²; Laura Tomlinson¹; Richard Gregory¹; Kevin Colizza³; Alexandr Muck⁴; ¹GSK, Stevenage, United Kingdom; ²Waters Corporation, Wilmslow, United Kingdom; ³GSK, Collegeville, PA; ⁴Waters Corporation, Wilmslow, United Kingdom
- WP 162 **Pharmacokinetics of Ketamine Transfer into Human Milk;** Palika Datta¹; Kaytlin Krutsch¹; Teresa Baker¹; Thomas Hale¹; ¹Texas Tech University Health Sciences Center, Amarillo, TX
- WP 163 **Mass spectrometry analysis of the contradiction between antiparasitic protection and immune responses in a Chagas disease nonhuman primate vaccination model;** Zongyuan Liu¹; Priscila Silva Grijó Farani²; John L. Vandenberg³; Igor C. Almeida²; Laura-Isobel McCall¹; ¹Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK; ²Border Biomedical Research Center, University of Texas El Paso, El Paso, TX; ³Department of Human Genetics, South Texas Diabetes and Obesity Institute, Edinburg, TX
- WP 164 **Development of an Ion Mobility CCS Database for Detection of Quaternary Ammonium Compounds and their Hepatic Phase I Human Metabolites;** Ryan Nguyen¹; Ryan P Seguin¹; Libin Xu¹; ¹University of Washington, Seattle, WA
- WP 165 **Multi-Elemental Detection of Heteroatoms for Standard-Free Quantitation of Xenobiotics;** Grace E Hahn¹; Frenio A Redeker¹; Kaveh Jorabchi¹; ¹Georgetown University, Washington, DC
- WP 166 **Metabolism study of the novel cathinone derivative 3-MMC combining three in vitro approaches, LC-HRMS acquisition and molecular networking tools;** Eliès Zarrouk¹; Alan Barnes²; Stephane Moreau³; Neil Loftus²; Sylvain Dulaurent¹; Souleiman Elbalkhi¹; Franck Saint-Marcoux¹; ¹CHU Limoges, Limoges, France; ²Shimadzu Corporation, Manchester, United Kingdom; ³Shimadzu Europa GmbH, Duisburg, Germany
- WP 167 **Optimization of the Ion Source-Mass Spectrometry Parameters Using High Throughput Rapidfire Mass Spectrometry and Design of Experiments Approach;** Timothy Schwemler¹; Hoorah Shaghaghi¹; ¹Alliance Pharma Inc, Malvern, PA
- WP 168 **Improved Quantitation of Sulfated Compounds in Human Plasma and Urine through Hydrolysis with Purified Arylsulfatase;** Amanda C. McGee¹; Douglas Waites¹; L. Andrew Lee¹; ¹Integrated Micro-chromatography Systems, Inc, Irmo, SC
- WP 169 **Bioanalytical Support for a Single-Arm Human Mass Balance and Absolute Bioavailability Study for Inavolisib using a Stable Labeled IV Microtracer;** Ryan Johnson¹; Xiaorong Liang¹; Brian Dean¹; Shuguang Ma¹; Sungjoon Cho¹; ¹Genentech Inc, South San Francisco, CA
- WP 170 **Enhancing Structural Elucidation of Drug-related Metabolites by Coupling Ion Mobility and Site-of-Metabolism Collision Cross-Section Predictions;** Jarod Fincher¹; Ismael Zamora²; Mark Cancilla¹; ¹Merck & Co., West Point, PA; ²Lead Molecular Design, S.L., Sant Cugat del Valles, Spain
- WP 171 **Investigation of fenebrutinib metabolism and bioactivation pathways via tandem-in-time fragmentation in an Ion Trap MS;** Aishah M Alsibae¹; Ali S Abdelhameed¹; Mohamed W. Attwa¹; Adnan A Kadi¹; ¹College of Pharmacy, King Saud University, Riyadh, SA, Riyadh, Saudi Arabia
- WP 172 **Investigation of in-vitro potential toxic metabolite formation for some selected tyrosine kinase inhibitors;** Abdulaziz Aljohari¹; Adham Bahian¹; Adnan A Kadi¹; A. F. M. Motiur Rahman¹; ¹King Saud University, Riyadh, Saudi Arabia
- WP 173 **Polymer StudioTM: a novel software for fast profiling and identifying complex pharmaceutical excipients by UHPLC-HRMS/MS technique;** Zhe Wang¹; Jiamin Gao²; Xinjian Li¹; Yanan Wang¹; Ning Sheng¹; Runtao Tian²; Jinlan Zhang¹; ¹Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing, China; ²Chemmind Technologies Co., Ltd., Beijing, China
- WP 174 **Unraveling sequences of impurities and degradants of a non-linear therapeutic peptide using a high-resolution LC-MS/MS workflow with electron-activated dissociation;** Eva Duchoslav¹; Harini Kaluarachchi¹; Giulia Calloni²; ¹SCIEX, Concord, ON; ²SCIEX, Darmstadt, Germany
- WP 175 **Method Translation from EI GC/HRMS to Atmospheric Pressure Ionization GC/MS/MS: Quantitative Analysis of Organochlorine Pesticides in Biota;** Douglas Stevens¹; Lindsay Hatch¹; Sarah Dowd¹; Frank Dorman¹; ¹Waters, Milford, MA
- WP 176 **A Quick MRM Method for FASAs Analysis in Surface Water Using UHPLC-MS/MS;** Danyang Wang¹; Vanisree Mulabagal¹; Meredith Feltman¹; Roger Viticoski¹; Joel Hayworth¹; ¹Auburn University, Auburn, AL
- WP 177 **A Compound Discoverer workflow integrated with molecular networking enables non-targeted class-based separation of Per- and polyfluoroalkyl substances (PFAS) homologous series;** Juan M Sanchez¹; Ralf Tautenhahn²; ¹ThermoFisher Scientific, Redwood City, CA; ²ThermoFisher Scientific, San Jose, CA
- WP 178 **Total Fluorine Quantitation by Plasma Assisted Reaction Chemical Ionization Mass Spectrometry;** Samuel R White¹; Kaveh Jorabchi¹; ¹Georgetown University, Washington, DC
- WP 179 **A Comparison of Liquid-Liquid Extraction and Stir Bar Sorptive Extraction for the Analysis of Organo-Iodides using GCxGC High-Resolution Mass Spectrometry;** Caroline O. Granger¹; Heather A. Brant¹; Haley B. Lawton¹; Stephanie N. Gamble¹; Amie C. McElroy¹; Joseph M. Mannion¹; ¹Savannah River National Laboratory, Aiken, SC
- WP 180 **Determination of reference values for PFAS in a wide variety of biotic and abiotic commercially available reference materials;** Camden Camacho¹; John A. Bowden¹; ¹University of Florida, Chemistry Department, Analytical Chemistry Division, Gainesville, FL
- WP 181 **Online LC / 21T FT-ICR MS and ICP-MS Analysis of Dissolved Organic Matter (DOM);** Ryan P Rodgers^{1, 2, 3, 4}; Martha L. Chacón-Patiño^{1, 5}; Win Robbins¹; Deisy Giraldo⁴; Joseph Frye-Jones²; Chad Weisbord¹; Alan G Marshall^{1, 2}; Brice Bouyssiere^{4, 5}; Pierre Giusti^{5, 6}; ¹National High Magnetic Field Laboratory, Tallahassee, FL; ²Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; ³International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harfleur, France; ⁴Université de Pau et des Pays de l'Adour, Pau, France; ⁵International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harfleur, France; ⁶TotalEnergies OneTech R&D, TotalEnergies Research & Technology, Gonfreville, France

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- WP 182 **Streamlining EPA Method 8270E Adoption Using the Verified Method Approach**; Thomas Dillon; *PerkinElmer, Shelton, CT*
- WP 183 **PH EFFECTS ON SOLID PHASE EXTRACTABLE DISSOLVED ORGANIC MATTER: EXPANDING THE ANALYTICAL WINDOW**; Justin Elliott¹; Hussain A Abdulla¹; ¹*Texas A&M Corpus Christi, corpus christi, TX*
- WP 184 **High sensitivity quantification and mass distribution analysis of microplastics in water using single particle ICP-MS**; Andrew P Fornadel¹; Tomoko Vincent²; Dhinesh Asogan²; Daniel Kutscher²; Jon Peters³; Matthew Cassap⁴; ¹*Thermo Fisher Scientific, Severna Park, MD*; ²*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*; ³*Thermo Fisher Scientific, Austin, Texas*; ⁴*Thermo Fisher Scientific, Runcorn, United Kingdom*
- WP 185 **N-dealkylation reactions of amines during water disinfection: new direction in the formation of DBPs**; Dmitrii Mazur¹; Sergey Sypalov²; Il'ya Varsegov²; Artiom Surmillo¹; Nikolay V Ul'yanovskii²; Dmitry S. Kosyakov²; Albert T Lebedev¹; ¹*Moscow State University, Moscow, Russian Federation*; ²*Lomonosov Northern (Arctic) Federal University, Core facility "Arctica", Arkhangelsk, Russia*
- WP 186 **Non targeted analysis of VOCs in new build homes using pyrolysis-GC/MS and solid phase extraction elements**; Khadiza Mom; *Quantum Analytics, The Woodlands, TX*
- WP 187 **Rapid and sensitive detection of per- and polyfluoroalkyl substances (PFASs) via bubbling and mass spectrometry**; Chuping Lee; *Department of Chemistry, National Chung Hsing University, Taichung, Taiwan*
- WP 188 **Characterising biosurfactants produced by Bacillus humi using LC MS/MS**; Bello A. Abubaker¹; Jim H Scrivens¹; Chris Ennis¹; Jackie A Mosely²; ¹*School of Health and Life Sciences, Teesside University, Middlesbrough, United Kingdom*; ²*University of York, York, United Kingdom*
- WP 189 **Identification of endocrine disrupting chemicals in human urine using non-targeted analysis**; Anca Baesu¹; Yong-Lai Feng¹; ¹*Health Canada, Ottawa, ON*
- WP 190 **UV-induced photodegradation of emerging para-phenylenediamine quinones in aqueous environment**; Wei Wang¹; Guodong Cao¹; Jing Zhang¹; Han Qiao¹; Huankai Li¹; Yanyan Chen¹; Yuecheng Sang¹; Zongwei Cai¹; ¹*Hong Kong Baptist University, Hong Kong, China*
- WP 191 **An alternative approach for ASTM D7845 in determining chemical species in Marine fuel oil by Gas Chromatography/Mass Spectrometry**; Jessin Mathai¹; Shailesh Sadashiv Damale¹; Atul Narkar¹; Kumar Raju¹; Rajendra Makhamale¹; ¹*Shimadzu Middle East & Africa FZE, Dubai, United Arab Emirates*
- WP 192 **The effect of environmentally relevant concentrations of atorvastatin, lovastatin, and simvastatin on Eisenia hortensis**; Kendra G. Selby¹; Gabriel A. Bressendorff¹; Lauren H. Phan¹; Noah E. Hanratty¹; Sydney R. Worth¹; Tyson A. Lobb¹; Hannah A. Konschak¹; Claire E. Korte¹; Carolyn J. Butts-Wilmsmeyer¹; Kevin R. Tucker¹; ¹*Southern Illinois University Edwardsville, Edwardsville, IL*
- WP 193 **Real-Time Monitoring of PFAS in Air with PTR-MS**; Christian Lindinger¹; Alfons Jordan¹; Tobias Reinecke¹; Rene Gutmann¹; Andreas Mauracher¹; Jens Herbig¹; Lukas Märk¹; Todd Rogers²; Philipp Sulzer¹; ¹*IONICON Analytik GmbH, Innsbruck, Austria*; ²*Trace VOC, Kennewick, WA*
- WP 194 **Characterization of protein and pharmaceutical profiles in wastewater by mass spectrometry for wastewater based epidemiology and water quality monitoring**; Montserrat Carrascal¹; Mira Čelić^{2,3}; Ester Sánchez-Jiménez¹; Antoni Ginebreda⁴; Joaquín Abian¹; Mira Petrović^{5,6}; M. José Farré^{2,3}; Damià Barceló^{4,5}; ¹*Biological and Environmental Proteomics, Institute of Biomedical Research of Barcelona, Spanish National Research Council, Barcelona, Spain*; ²*Water Quality Area, Catalan*
- Institute for Water Research (ICRA), Girona, Spain*; ³*University of Girona, Girona, Spain*; ⁴*Water and Soil Quality Research Group, Department of Environmental Chemistry, IDAEA-CSIC, Barcelona, Spain*; ⁵*Catalan Institute for Water Research (ICRA), Girona, Spain*; ⁶*Catalan Institution for Research and Advanced Studies (ICREA), Barcelona, Spain*
- WP 195 **Specific determination of non-ionic surfactants in drinking-, waste- and surface water with high resolution mass spectrometry**; Dennis JA Van Den Heuvel¹; Johan Scholtens¹; Tamara Haagsma¹; Stephane Moreau²; ¹*Shimadzu Benelux, 's-Hertogenbosch, Netherlands*; ²*Shimadzu Europa GmbH, Duisburg, Germany*
- WP 196 **Explosive analysis in soil at 8 Seconds per Sample Using the LDTD-MS/MS**; Jonathan Rochon¹; Serge Auger¹; Jean Lacoursière¹; Pierre Picard¹; ¹*Phytronix Technologies Inc., Québec, QC*
- WP 197 **Using TOCA PIMS as a tool for investigating emissions from residential heating by brown coal briquettes and other aerosols sources**; Patrick Martens¹; Hendryk Czech¹; Olli Sippulla²; Sven Ehlert³; Andreas Walte³; Ralf Zimmermann¹; ¹*Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany*; ²*University of Eastern Finland, Department of Environmental and Biological Sciences, Fine Particle and Aerosol Technology Laboratory, Kuopio, Finland*; ³*Photonion GmbH, Schwerin, Germany*
- WP 199 **Analysis of Nonylphenols and Phthalates from Food Contact Packaging using GC/MS/MS**; Matthew Curtis¹; David A Weil²; ¹*Agilent Technologies, Santa Clara, CA*; ²*Agilent Technologies, Inc., Santa Clara, CA*
- WP 200 **Screening for extractables and leachables in nasal spray devices using high-resolution mass spectrometry combined with a data independent informatics strategy**; Richard Lock¹; Rachel J Sanig²; Sarah Dowd³; Lee Gethings⁴; Nick Morley⁵; ¹*Waters Corporation, Wilmslow, United Kingdom*; ²*Waters Corporation, Wilmslow, United Kingdom*; ³*Waters Corporation, Milford, MA*; ⁴*Waters, Wilmslow, United Kingdom*; ⁵*Element Materials Technology, Wythenshawe, United Kingdom*
- WP 201 **Enhanced Extractable Leachable Compound Identification using New Database Software with Retention Time and Supplemental Collisional Cross Sections**; David A Weil¹; Andrew McEachran¹; Cate Simmermaker¹; Sarah Stow¹; ¹*Agilent Technologies, Santa Clara, CA*
- WP 202 **The Role of Mass Spectrometry in the Circular Economy of Plastics. Deconvolution of Mass-Spectral-Data Derived from Extracts of Polymer Mixtures**; Yamil Simón-Manoso¹; Tytus D. Mak¹; Edward Erisman¹; Kelly H. Telu¹; Xiaoyu Yang¹; Yuxue Liang¹; William E. Wallace¹; Stephen E. Stein¹; ¹*NIST, Gaithersburg, MD*
- WP 203 **Characterizing Extractables from Common Pharmaceutical Packaging Materials by High Resolution Time of Flight Mass Spectrometry and Enhanced Gas Chromatography Separations**; Elizabeth Humston-Fulmer¹; David E Alonso¹; Joseph E Binkley¹; ¹*LECO, St. Joseph, MI*
- WP 204 **Extractables and Leachables Testing of Plastic Water Bottles and Their Contents using VASE and Flash-VASE Sample Preparation and GCMS Analysis**; Daniel Cardin¹; Weiwei Hao¹; John Quintana¹; ¹*Entech Instruments, Simi Valley, CA*
- WP 205 **High-Throughput Characterization of Fentanyl Analogs using LC-TIMS-TOF MS/MS**; Andrew R Forero¹; Lilian Valadares Tose¹; Matthew Willetts²; Melvin A. Park²; Francisco Alberto Fernandez Lima^{1,3}; ¹*Department of Chemistry and Biochemistry, Florida International University, Miami, FL*; ²*Bruker Daltonics Inc., Billerica, Massachusetts*; ³*Biomolecular Sciences Institute, Florida International University, Miami, Florida*

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- WP 207 **Rapid GC-MS and Solid-Phase Microextraction as a Screening Method for Forensic Fire Debris Applications;** Briana A. Capistran; National Institute of Standards and Technology, Gaithersburg, MD
- WP 208 **Target compounds for mass spectrometry imaging after Fingerprint Enhancement Techniques;** Mariska Banidol¹; Sophia Kouider²; H el ene Pizzala²; Laurence Charles²; ¹Aix Marseille Universit e, CNRS, Institut de Chimie Radicalaire, MARSEILLE, France; ²Aix Marseille Universit e, CNRS, Institut de Chimie Radicalaire,, MARSEILLE, France
- WP 209 **Detection of post-blast triacetone triperoxide (TATP) by 3D-printed cone spray, DART, and SPME-GC-MS: a comparison for forensic casework;** Ryan M. Bain¹; Patrick W. Fedick²; Tj Pinedo; Christopher C. Mulligan³; Shane Kullen¹; Gui-hua Lang¹; Douglas J. Klapac¹; ¹Bureau of Alcohol, Tobacco, Firearms and Explosives, Beltsville, MD; ²Naval Air Warfare Center, United States Navy Naval Air Systems Command (NAVAIR), China Lake, CA; ³Illinois state university, Normal, IL
- WP 210 **Recovery and Detection of Fentanyl Analogs and Precursors from Shipping Materials by Pressure-Sensitive Adhesive and Paper Spray-Mass Spectrometry;** Sarah Prunty¹; Nicholas Manicke²; Elizabeth Dhummakupt³; Dan Carmany⁴; ¹Indiana University-Purdue University Indianapolis, Indianapolis, IN; ²Indiana University Purdue University Indianapolis, Indianapolis, IN; ³U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; ⁴EXCET Incorporated, Edgewood, MD
- WP 211 **Average Signal Intensities from Qualitative Large-Scale Trace-Residue Analysis of Discarded Drug Paraphernalia Provide Quantitative Information on Dynamic Illicit Drug Markets;** Henry West¹; Michael G Leeming¹; Gavin E Reid¹; ¹University of Melbourne, Parkville, Australia
- WP 212 **Differentiation of Hemp and Marijuana Using Ag-Ligand Ion Complexation and a Semi-Quantitative Decision-Point Assay;** Alleigh N. Couch¹; Jayleigh M. Lanza²; Christopher M. Zall²; J. Tyler Davidson¹; ¹Department of Forensic Science, Sam Houston State University, Huntsville, TX; ²Department of Chemistry, Sam Houston State University, Huntsville, TX
- WP 213 **Over-The-Counter sex wellness products screening using a portable/field deployable MS equipped with a Direct Sampling Atmospheric Pressure source;** Enrico Davoli¹; Alice Passoni¹; Claudio Medana²; Enrica Mecarelli²; Victor Laiko³; Vladimir Doroshenko³; ¹Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy; ²Universita' degli Studi di Torino, Torino, Italy; ³MassTech Inc, Columbia, MD
- WP 214 **Toward Improved Isomers Separation through Reductive Amination in Synthetic Cathinone, take 4-Methylethcathinone, 4-Ethylmethcathinone and 4-methyl-N,N-dimethylcathinone as an example;** Shih-Shin Liang; Kaohsiung Medical University, Kaohsiung, Taiwan
- WP 215 **Differentiation of synthetic sources of an organophosphorus chemical by LC-MS-based metabolomics;** Carla Orlandi^{1,2}; Gr egoire Delaporte³; Christine Albaret³; Emmanuel Joubert³; Anne Boss e⁴; Laurent Debrauwer^{1,2}; Emilien L Jamin^{1,2}; ¹Toxalim (Research Center in Food Toxicology), Toulouse university, INRAE, ENVT, INP-Purpan, Toulouse, France; ²MetaboHUB-MetaToul, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France; ³Analytical Chemistry Department, DGA CBRN Defence, 5 rue Lavoisier, Vert-Le-Petit, France; ⁴Chemistry Division, DGA CBRN Defence, 5 rue Lavoisier, Vert-Le-Petit, France
- WP 216 **Investigating the utility of hybrid similarity scores with mass spectra collected using DART-MS: A case study with PCP analogs;** Edward Sisco¹; Arun Moorthy¹; ¹NIST, Gaithersburg, MD
- WP 217 **Liquid Chromatographic High Resolution Accurate Mass Characterization of Polydimethylsiloxanes on Condoms and Sexual Lubricants;** B. Mckay Allred¹; James Adams¹; Joshua Little²; ¹USACIL, Forest Park, GA; ²ORISE - USACIL, Forest Park, GA
- WP 218 **HR-MS/MS as a way to avoid false positive quantification of 27 psychoactive compounds in venous and VAMS-collected blood;** Julia Mironenka¹; Anna Lenartowicz¹; Adrian Sobo n^{1,2}; Rafa l Szewczyk^{1,2}; Katarzyna Krupczy nska-Stopa^{1,2}; Maciej Stopa^{1,2}; Andrzej Kwa nsnica³; ¹LabExperts sp. z o. o., Gda nsk, Poland; ²Bioanalytic sp. z o. o., Gda nsk, Poland; ³Lab4Tox sp. z o. o., Wroclaw, Poland
- WP 219 **Molecular investigation of benzodiazepines in human blood by DART ionization and High-Resolution Mass Spectrometry;** Cecilia A. Bhering¹; Ananda S. Antonio¹; Gleicielle T. Wurzler¹; Alexandre N. P. Aguiar¹; Diego R. Carvalhosa²; Ant nio C. G. Jardim³; Marc Y. Chalom^{3,4}; Francois Espourteille⁵; Julio C. G. Silva⁶; Francisco R. A. Neto¹; Gabriela V. Costa¹; ¹Universidade Federal do Rio de Janeiro, Instituto de Qu mica, NAF - LADETEC, Rio de Janeiro, Brazil; ²PCERJ, SEPOL, Instituto M dico Legal Afr nio Peixoto (IMLAP), Rio de Janeiro, Brazil; ³SENS Advanced Mass Spectrometry, S o Paulo, Brazil; ⁴Consultancy, S O PAULO, Brazil; ⁵Bruker Scientific, Billerica, MA; ⁶Nova Anal tica, S o Paulo, Brazil
- WP 220 **Application of DART ionization in the forensic investigation of pesticide poisoning;** Gleicielle T. Wurzler¹; Ananda S. Antonio¹; Cecilia A. Bhering¹; Thamara A. Barra¹; Alexandre N. P. Aguiar¹; Diego R. Carvalhosa²; Ant nio C. G. Jardim³; Marc Y. Chalom^{3,4}; Julio C. G. Silva⁵; Francois Espourteille⁶; Francisco R. A. Neto¹; Gabriela V. Costa¹; ¹Universidade Federal do Rio de Janeiro, Instituto de Qu mica, NAF - LADETEC, Rio de Janeiro, Brazil; ²PCERJ, SEPOL, Instituto M dico Legal Afr nio Peixoto (IMLAP), Rio de Janeiro, Brazil; ³SENS Advanced Mass Spectrometry, S o Paulo, Brazil; ⁴Consultancy, S O PAULO, Brazil; ⁵Nova Anal tica, S o Paulo, Brazil; ⁶Bruker Scientific, Billerica, MA
- WP 221 **Application of Machine-learning to Predict Physical Activity from Endogenous Fingerprint Compounds;** Daphne R. Patten¹; Trevor T Forsman¹; Andrew E Paulson¹; Young Jin Lee¹; ¹Iowa State University, Ames, IA
- WP 222 **Using High Resolution Mass Spectrometry to clarify ambiguous Benzodiazepine ions in the NIST EI-MS Library;** Edward Erisman¹; Arun Moorthy¹; William E. Wallace¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD
- WP 223 **Comparing Peptide Sequence Accuracy of MRM to Peptide Spectra Searching;** Hevi Yang¹; Erin Butler¹; Iyman Almubarak¹; Tatiana Perez¹; Jahaira Zapata¹; Donald Siegel¹; ¹Office of Chief Med Exam, New York, NY
- WP 224 **Enhanced Ultra-Sensitive Detection of Explosives Through Thermal Desorption Filters Sampling and Multi-Scheme Ambient Pressure Chemical Ionization Source (MION);** Elie Lattouf¹; Aleksei Shcherbinin²; Juha Kangasluoma^{2,3}; Paxton Juuti²; Jussi Kontro²; Joona Mikkil ²; Jyri Mikkil ²; H.j. Jost²; ¹Research scientist/Scientific Sales Lead, Helsinki, Finland; ²Karsa Ltd., Helsinki, Finland; ³Institute for Atmospheric and Earth System Research (INAR), University of Helsinki, Helsinki, Finland
- WP 225 **Open Port Sampling Interface (OPSI) with a Compact Mass Spectrometer for Trace Contraband Detection;** Shin Muramoto; National Institute of Standards and Technology, Gaithersburg, MD

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- WP 226 **Van de Graaff generators as combined sampling devices and ion sources for non-contact mass spectrometry analysis of evidentiary materials;** Kenyon Evans-Nguyen¹; Madison Autrey¹; ¹University of Tampa, Tampa, FL
- WP 227 **Rapid Characterization of Alkaloids using Probe ESI-Q-TOF LCMS-9050 in OAD-MS/MS;** Hidenori Takahashi¹; Kaoru Nakagawa¹; Mami Okamoto¹; Yuta Miyazaki¹; Yohei Arai¹; Tetsuo Iida¹; ¹SHIMADZU Corporation, Kyoto, Japan
- WP 228 **High-speed analysis of drugs of abuse in urine using Acoustic Ejection Mass Spectrometry;** Anuja Bhalkikar¹; Jacob Watson McCabe¹; Han Joo Lee¹; Rahul Baghla²; Casey W. Burrows¹; Alexandre Wang¹; ¹SCIEX, Frammingham, MA; ²SCIEX, Redwood city, CA
- WP 229 **Generic extraction method developed for the screening of whole blood at 8 Seconds per Sample Using the LDTD-MS/MS;** Sylvain Letarte¹; Hugues Sinnett¹; Serge Auger¹; Jean Lacourcière¹; Jonathan Rochon¹; Pierre Picard¹; ¹Phytronix Technologies, Quebec, QC
- WP 230 **Extraction of Illicit Drugs from Wastewater using a Solid Phase Extraction Syringe-cartridge Capsule;** Michael Apsokardu¹; Xiaohui Zhang¹; Guotao Lu¹; ¹CDS Analytical, Oxford, PA
- WP 231 **An Innovative Approach to QTOF High Resolution Accurate Mass Analyte Screening Using an Improved Software Algorithm and Screener Tool;** Peter Stone; Agilent Technologies, Santa Clara, CA
- WP 232 **Characterization of lipoprotein subclasses using Orbitrap charge detection mass spectrometry;** James D. Sanders¹; Kimber N. Focke²; Michael T Marty²; ¹University of Arizona, Tucson, AZ; ²University of Arizona, Tucson, AZ
- WP 233 **Architecture of Adeno-Associated Viral Capsids with Surface-Induced Dissociation and Charge Detection Mass Spectrometry;** Marius M Kostelic^{1,2}; Chen Du^{1,2}; Vicki H Wysocki^{1,2}; ¹Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; ²Resource for Native Mass Spectrometry-Guided Structural Biology, The Ohio State University, Columbus, OH
- WP 234 **Towards reference-free byproduct characterization of agrochemicals in raw plant extracts by ion spectroscopy;** Matthias Vink¹; Jonathan Martens¹; Wybren Jan Buma²; Giel Berden¹; Jos Oomens¹; ¹FELIX Radboud University, Nijmegen, Netherlands; ²University of Amsterdam, Amsterdam, Netherlands
- WP 235 **Identification of organic dye molecules using QIT-ToF-SIMS and photodepletion spectroscopy;** Chang Min Choi; Center for Scientific Instrumentation, Korea Basic Science Institute (KBSI), Cheongju-si, South Korea
- WP 236 **Towards routine annotation of mass spectral features with infrared ion spectroscopy;** Kas J. Houthuijs¹; Jonathan K. Martens¹; Giel Berden¹; Vasuk Gautam²; David S. Wishart²; Jos Oomens¹; ¹Radboud University Nijmegen, Nijmegen, Netherlands; ²University of Alberta, Edmonton, AB
- WP 237 **Design of an Optical Ion Trap (OIT) Mass Analyzer;** Liam Dugan¹; Frederick Lanni¹; Mark E Bier¹; ¹Carnegie Mellon University, Pittsburgh, PA
- WP 238 **A Quadrupole Time-of-Flight Mass Spectrometer with Off-Axis Ion Trap for Infrared Ion Spectroscopy in the Hydrogen Stretching Region;** Madeline Schultz¹; Neil A. Ellis¹; Maleesha T. Fernando¹; Miyuru M. Wellalage¹; Daniel A. Thomas¹; ¹University of Rhode Island, Kingston, RI
- WP 239 **Site-Specific Gas-Phase Acidities of Isoprene and the Negative Ion Photoelectron Spectra of C5H7 Radical Anions Resulting from Isoprene Oxidation;** Dushmantha N. Koku Hannadige Abevsooriya^{1,2}; Kie T. Workman^{1,3}; Wilson Gichuhi¹; ¹Department of Chemistry, Tennessee Tech University, 1 William L. Jones Dr., Cookeville, TN 38505; ²School of Environmental Studies, Tennessee Tech University, Cookeville, TN 38505; ³Department of Chemical Engineering, Tennessee Tech University, 1 William L. Jones Dr., Cookeville, TN 38505
- WP 240 **Action spectroscopy of triazole ions in the ultraviolet;** Alexandre Giuliani^{1,2}; Héloïse Dossmann³; Denis Duflot⁴; ¹Synchrotron Soleil, Gif-Sur-Yvette, France; ²INRAE, UAR1008, Transform Department, Rue de la Géraudière, BP 71627,44316 Nantes, France, Nantes, France; ³Sorbonne Université, Faculté des Sciences et de l'Ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France; ⁴Université de Lille, Laboratoire de Physique des Lasers, Atomes et Molécules, Villeneuve d'Ascq, France
- WP 241 **Gas Phase Intramolecular Photo Crosslinking in Tetrazole-Peptide Conjugates;** Jiahao Wan¹; Haocheng Qian¹; František Tureček¹; ¹University of Washington, Seattle, WA
- WP 242 **Identifying the Structural Properties of Choline-Chloride Deep Eutectic Solvents by Mass Spectrometry and Condensed-Phase Analysis;** Maleesha T Fernando¹; Miyuru M Wellalage¹; Emily M Molino¹; Madeline Schultz¹; Neil Ellis¹; Daniel A Thomas¹; ¹University of Rhode Island Chemistry Department, Kingston, RI
- WP 243 **Combining Mass Spectrometry and Condensed-Phase Analysis for the Structural Investigation of Hydrophobic Deep Eutectic Solvents;** Miyuru M Madduma Wellalage¹; Maleesha T Fernando¹; Emily M Molino¹; Madeline Schultz¹; Neil Ellis¹; Daniel A Thomas²; ¹University of Rhode Island, Kingston, RI; ²University of Rhode Island Chemistry Department, Kingston, RI
- WP 244 **Influence of the decavanadate oxidation state on its reactivity and structural dynamics in solution studied with 18O exchange.;** Daniel T Favre¹; Igor Kaltashov¹; ¹UMASS Amherst, Amherst, MA
- WP 245 **Exploring Emitters for Generating ultra-low Current Electrospray Ionization;** Ian T Ferraro¹; Huishan Li¹; Nicholas Allen¹; Taoqing Wang¹; Anyin Li¹; ¹Department of Chemistry, University of New Hampshire, Durham, NH
- WP 246 **Ionization Efficiency of Glycans, Proteins and Subunits in femto Electrospray Modes;** Huishan Li¹; Nicholas Allen¹; Taoqing Wang¹; Ian T Ferraro¹; Mengting Li¹; Anyin Li¹; ¹University of New Hampshire, Durham, NH
- WP 247 **Elevation of the baseline in Quadrupole Mass Spectrometers: Mechanism and Solution;** Markus Langner¹; Hendrik Kersten¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal, Germany
- WP 248 **Mapping Nano-Electrospray Ionization Plumes on an Orbitrap Fusion Lumos Tribrid Mass Spectrometer Equipped with FAIMS;** Joshua A Silveira¹; Gary A Schultz¹; Kristina Rucker¹; Yuan Lin¹; Matt Tsai¹; Michael Belford¹; Cornelia Boeser¹; Eloy R Wouters¹; ¹Thermo Fisher Scientific, San Jose, CA
- WP 249 **Uncatalyzed N-alkylation of Primary Amines via Plasma-Droplet Fusing Reactions: Quantification of Internal Energy Deposition and Product Collection;** Alexander J Grooms¹; Abraham K. Badu-Tawiah¹; ¹The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH
- WP 250 **Investigation of Long-Term Behavior of Large, Charged ESI Droplets Aspirated into the High Vacuum Region of two Commercial MS Systems;** Chris Vico Heintz¹; Oliver Braubach¹; Walter Wissdorf¹; Lisa Schnödewind¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal, Germany
- WP 251 **Observation of charged ESI droplets aspirated into the vacuum system of a commercial QIT under varied LC conditions;** Patricia Itzenhäuser¹; Laura Lehmann¹; Walter Wissdorf¹; Ferdinand Wachter¹; Hendrik Kersten¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal, Germany
- WP 252 **Investigating effects of supercharging reagents on signal intensity of peptides in negative ion mode using capillary vibrating sharp-edge spray ionization;** Amanda Devor¹; Jing Wang¹; Madison Pursell¹; Olanrewaju Awoyemi¹; Stephen Valentine¹; Peng Li¹; ¹West Virginia University- C. Eugene Bennett Department of Chemistry, Morgantown, WV

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- WP 253 **Gas-phase oxidation of benzaldehyde to benzoic acid under electrospray ionization mass spectrometric conditions;** Shimin He¹; Sihang Xu¹; Athula Attygalle¹; ¹*Stevens Institute of Technology, Hoboken, New Jersey*
- WP 254 **Thermal-Desorption Electrospray-Mass Spectrometry (TD-ESI-MS) for Dye Analysis;** Jiarui Rachel Wu¹; Xinyi Sui¹; Brian Musselman²; Nelson R Vinueza¹; ¹*North Carolina State University, Raleigh, NC*; ²*Bruker Scientific, Billerica, MA*
- WP 255 **Design and investigation of homemade argon plasma ion sources – An overview of source development, application, and ionization mechanism;** Florian Stappert¹; Alexandra Pape^{1,2}; Juan F. Ayala-Cabrera^{1,2,3}; Florian Uteschil^{1,2}; Oliver J. Schmitz^{1,2}; ¹*Applied Analytical Chemistry, University of Duisburg-Essen, Essen, Germany*; ²*Teaching and Research Center for Separation, University of Duisburg-Essen, Essen, Germany*; ³*Department of Analytical Chemistry, University of the Basque Country, Leioa, Spain*
- WP 256 **Measurement of Distribution of Ion Acceptance (DIA) in ESI and APCI ion sources;** Adem Bulut¹; Chris Vico Heintz¹; Walter Wissdorf¹; Thorsten Benter¹; ¹*University of Wuppertal, Wuppertal, Germany*
- WP 257 **Feeding the ALPACA: Testing the Performance of Charge-Induction Amperometry of Electrosprayed Particles;** Cristian A. Blanco-Combariza¹; Jeffrey E Dick²; ¹*Purdue University, West Lafayette, IN*; ²*Purdue University Department of Chemistry, West Lafayette, IN*
- WP 258 **Fast and Ultra Fast Lipids and Drugs Analysis in Whole Blood by GC-MS with Cold EI;** Benjamin Neumark¹; Oleg Elkabets¹; Aviv Amirav^{1,2}; ¹*Tel Aviv University, Tel Aviv, Israel*; ²*Aviv Analytical Ltd, Hod Hasharon, Israel*
- WP 259 **Solving Non-Linearity in GC-MS By Using Cold EI;** Alex Yakovchuk¹; Alexander Gordin¹; Aviv Amirav¹; ¹*Tel Aviv University, Tel Aviv, Israel*
- WP 260 **Open Probe Ultra-Fast GC-MS on the Bench for Improved Real Time Analysis;** Oleg Elkabets¹; Benny Neumark¹; Aviv Amirav^{1,2}; ¹*Tel Aviv University, Tel Aviv, Israel*; ²*Aviv Analytical Ltd, Hod Hasharon, Israel*
- WP 261 **Determination of six aromatic amines in the mainstream smoke of tobacco products;** Huihua Ji¹; Zhenyu Jin¹; ¹*University of Kentucky, Lexington, KY*
- WP 262 **Differential analysis of soil using GC Orbitrap MS and Compound Discoverer;** Dominic Roberts¹; Xin Zheng²; Lukasz Rajski³; Nicholas Warner³; Daniel Kutscher³; Jason Cole²; ¹*Thermo Fisher Scientific, Runcorn, United Kingdom*; ²*Thermo Fisher Scientific, Austin, Texas*; ³*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*
- WP 263 **Characterization of virgin and recycled industrial plastics using pyrolysis with soft ionization coupled to high-resolution mass spectrometry and statistical analysis;** Rachel J Sanig¹; Bryan C. Katzenmeyer²; Cristian Cojocariu¹; Jeff Goshawk¹; Agnieszka Kalinowska³; Christoph Rethmann³; Pascal Tuszewski³; Lindsay Hatch²; ¹*Waters Corporation, Wilmslow, United Kingdom*; ²*Waters Corporation, Milford, MA*; ³*thyssenkrupp Presta AG, Eschen, Liechtenstein*
- WP 264 **UPLC-MSMS Converted to an APGC-MSMS to Target Extremely Low Concentration Levels of Substances of Concern in Post-Consumer Recycled Resins;** Tianzi Huang¹; Snow Bai¹; Larry Shayne Greem¹; Peilin Yang¹; ¹*Dow, Inc., Lake Jackson, TX*
- WP 265 **Development and Evaluation of a Structural Analysis Method Using the EI Mass Spectrum Prediction Model by Machine Learning Technology;** Ayumi Kubo¹; Azusa Kubota¹; Masaaki Ubukata¹; Timothy Bergeron²; ¹*JEOL Ltd., Tokyo, Japan*; ²*JEOL USA, Inc., Peabody, MA*
- WP 266 **Structural Analysis of Polymer Materials Using Pyrolysis GC-HRTOFMS Data and a Predicted EI Mass Spectral Database Compiled by Machine Learning;** Azusa Kubota¹; Masaaki Ubukata¹; Ayumi Kubo¹; Kenji Nagatomo¹; John Gonzales²; ¹*JEOL Ltd., Tokyo, Japan*; ²*JEOL USA, Inc., Peabody, MA*
- WP 267 **Characterization of UV-degraded Polyethylene Terephthalate by Reactive-Pyrolysis GC-TOFMS and MALDI-TOFMS;** Takaya Satoh¹; Masaaki Ubukata¹; Azusa Kubota¹; Ayumi Kubo¹; Robert A. Dipasquale²; ¹*JEOL Ltd., Tokyo, Japan*; ²*JEOL USA, Inc., Peabody, MA*
- WP 268 **Untargeted screening and identification of substances in plastic food contact materials using an Orbitrap GC mass spectrometer;** Dominic Roberts¹; Jason Cole²; Lukasz Rajski³; Xin Zheng²; Pablo Miralles⁴; Clara Coscolla⁴; ¹*Thermo Fisher Scientific, Runcorn, United Kingdom*; ²*Thermo Fisher Scientific, Austin, Texas*; ³*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*; ⁴*Foundation for the Promotion of Health and Biomedical Research in the Valencian Region (FISABIO-Public Health), Valencia, Spain*
- WP 269 **Simultaneous determination of fatty acids in commercial lipid samples by gas chromatography coupled with single quadrupole mass spectrometry (GC-SQMS);** Mark Dennis Chico Retrato^{1,2}; Siyuan Qiu¹; Anna Lundquist²; Aida Zuberovic Muratovic³; Kumari Ubhayasekera¹; Jonas Bergquist¹; ¹*Department of Chemistry - Biomedical Center, Analytical Chemistry and Neurochemistry, Uppsala University, Uppsala, Sweden*; ²*Innovation and Development Department, Fresenius-Kabi, Uppsala, Sweden*; ³*Swedish Food Agency (Livsmedelsverket), Uppsala, Sweden*
- WP 270 **Operational Fundamentals and Optimization of Vacuum-Assisted Headspace Solid Phase Microextraction for Gas Chromatography Analysis of Solid Samples;** Shannon L. Thomas¹; Colton Myers²; Jason Herrington²; Kevin A. Schug¹; ¹*University of Texas at Arlington, Arlington, TX*; ²*Restek Corporation, Bellefonte, PA*
- WP 271 **More Than 43,400 High Quality Spectra Added to a Comprehensive Electron Ionization (EI) Mass Spectral Library;** Weihua Ji¹; Lewis Y. Geer¹; Nirina Rabe Andriamaharavo¹; Yufang Zheng¹; Edward P. Erisman¹; H. Martin Garraffo¹; James Little¹; Gary Mallard¹; Sanford P. Markey¹; Yuri A. Mirokhin¹; Quan-Long Pu¹; Dmitrii V. Tchekhovskoi¹; Nino G. Todua¹; Oleg V. Toropov¹; Kirill V. Tretyakov¹; William E. Wallace¹; Stephen E. Stein¹; ¹*NIST, Gaithersburg, MD*
- WP 272 **Using Hydrogen as Carrier Gas for GC/MS Analysis: GCxGC-HR-TOFMS with Multi-Mode Ion Source;** George Tikhonov¹; Scott Pugh¹; Vyacheslav Artaev¹; ¹*LECO Corporation, Saint Joseph, MI*
- WP 273 **Rearrangement of the TMS ester of 4-Difluoromethoxy-N-methylbenzylamine and analogs in EI mass spectra;** Quan-Long Pu¹; Yufang Zheng¹; Kirill V. Tretyakov¹; Edward P. Erisman¹; ¹*NIST, Gaithersburg, MD*
- WP 274 **Measurement and Evaluation of Plant Derived Compounds for a Comprehensive Electron Ionization MS Library;** Nirina Rabe Andriamaharavo¹; Mak D. Tytus²; Weihua Ji¹; William E. Wallace²; Stephen E. Stein¹; ¹*National Institute of Standards and Technology, Gaithersburg, MD*; ²*National Institute for Standards and Technology, Gaithersburg, MD*
- WP 275 **Full Evaporative Vacuum Extraction – A Quantitative and Green Approach for Analysis of Semivolatile Organic Compounds in Water Using GC-MS;** Weier Hao¹; Dan Cardin¹; John Quintana¹; Tim Raub¹; ¹*Entech Instruments, Simi Valley, CA*
- WP 276 **Analysis of Volatile and Semivolatile Organic Compounds in Oral Rinse using Vacuum Assisted Sorbent Extraction and GC-MS;** Tim Raub¹; Dan Cardin¹; Weier Hao¹; John Quintana¹; ¹*Entech Instruments, Simi Valley, CA*
- WP 277 **Helium to Hydrogen: Explosives & Pesticides & VOAs, Oh My! Successful Transition of GC/MS Analyses;** Eric Fausett¹; Anastasia Andrianova²; Bruce Quimby³; Angela

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- Smith Henry³; Kirk Lokits²; Limian Zhao²; Jessica Westland⁴; Samuel P Haddad⁴; Aaron Boice⁵; ¹Agilent, Landenberg, PA; ²Agilent Technologies, Wilmington, DE; ³Agilent Technologies, Wilmington, Delaware; ⁴Agilent Technologies, Wilmington; ⁵Agilent Technologies, Santa Clara, CA
- WP 278 **Large Volume Static Headspace for Flavor/Fragrance Analysis by GC-MS Using Novel Hybrid Capillary/Packed Sorbent Traps;** John Quintana¹; Dan Cardin¹; Weier Hao¹; Tim Raub¹; ¹Entech Instruments, Simi Valley, CA
- WP 279 **Analysis of Hop Oil Chemical Composition using GC/MS-SCD to Quantitate Essential Oil from 3 PPM -1 w/w%;** Lupe Saldana¹; Jacqueline Brummett¹; Patrick Jensen¹; ¹Yakima Chief Hops - Yakima, WA, Yakima, WA
- WP 280 **Bench Scale Py-GC/MS with In-Line Reactor for Predicting Arrhenius Parameters;** Jeffrey Michael McGuire¹; John C Carpin²; ¹U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; ²EXCET Incorporated, Edgewood, MD
- WP 281 **Internal standards for optimization of precision and accuracy of an automated liquid handler for hydrogen exchange-mass spectrometry (HX-MS);** Ekaterina Deyanova¹; David Weis¹; ¹Bristol-Myers Squibb, Princeton, NJ
- WP 282 **An Improved Apparatus with On-Line Chromatography for Hydrogen Deuterium Exchange Mass Spectrometry Measurements from Milliseconds to Hours;** Joseph Anacleto^{1, 2}; Cristina Lento²; Ayesha Maqsood²; Derek Wilson²; ¹Emeritus, Brampton, ON; ²York University, Toronto, ON
- WP 283 **Development and Application of Spray-capillary to Room Temperature Hydrogen-Deuterium Exchange for Top-Down Mass Spectrometry Applications;** Joel B Langford¹; Mulin Fang¹; Kellye A. Cupp-Sutton¹; Jake Kline¹; Luca Fornelli¹; Si Wu¹; ¹University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK
- WP 284 **HILIC separations for HDX-MS at subzero temperatures;** Kyle W Anderson¹; Jeffrey W Hudgens¹; ¹NIST, Rockville, MD
- WP 285 **deMix_GUI: A software package for automated HDX-MS data analysis and interrogation;** Hyeyun Jung¹; Seungjin Na²; Eunok Paek²; ¹Grinnell College, Grinnell, IA; ²Hanyang University, Seoul, South Korea
- WP 286 **Development of a PNGase Rc column for efficient online deglycosylation of complex glycoproteins during HDX-MS;** Thomas Ole Tandrup Lambert¹; Marius Gramlich²; Luke Smith³; Luisa Stutzke¹; Dingyu Deng¹; Philipp Kaiser²; Alesi Escobedo⁴; Ellie James⁴; Mike Guttman⁴; Justin LP Benesch³; Ulrich Rothbauer²; Maximiliane Koenig⁵; Cornelia Wagner⁵; Pavla Vankova⁶; Petr Pompach⁶; Petr Novak⁷; Anne Zeck²; Kasper D. Rand¹; ¹Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; ²NMI Natural and Medical Sciences Institute at the University of Tübingen, Reutlingen, Germany; ³Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom; ⁴Department of Medicinal Chemistry, University of Washington, Seattle, Washington; ⁵Roche Pharma Research and Early Development, Large Molecule Research, Penzberg, Germany; ⁶BioCeV - Institute of Biotechnology of the CAS, Prague, Czech Republic; ⁷BioCeV - Institute of Microbiology of the CAS, Prumyslova, Czech Republic
- WP 287 **Development of a thiol-ene microfluidic chip for sub-zero temperature hydrogen/deuterium exchange mass spectrometry (HDX-MS);** Anton B. Hansen¹; Rasmus R. Svejdal¹; Jack Barrett¹; Jörg P. Kutter¹; Kasper D. Rand¹; ¹Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark
- WP 288 **Differential HX-MS of complex drug targets extracted from cells: a full solution using HX-DIA technology;** František Filandr¹; Vladimir Sarpe¹; Shaunak Raval¹; Morgan Khan¹; Pauline Douglas¹; Yuqi Shi²; Rosa Viner²; Stephen Coales³; David Schriemer¹; ¹University of Calgary, Calgary, AB; ²Thermo Fisher Scientific, San Jose, CA; ³Trajan Scientific & Medical - Raleigh, Morrisville, NC
- WP 289 **A fully automated HX-DIA data analysis workflow for whole proteome deuteration experiments;** Vladimir Sarpe¹; František Filandr¹; D Alex Crowder¹; David C Schriemer¹; ¹University of Calgary, Calgary, AB
- WP 290 **Histidine hydrogen-deuterium exchange (His-HDX) mass spectrometry for identifying protein-ligand interactions;** Kouhei Tanaka¹; Tarou Kishimoto¹; Shinko Watanabe¹; Kaori Mitsui¹; Chieko Okumura¹; Kouta Murasaki¹; Masaru Miyagi²; Ayako Kurimoto³; Sen Ilker³; ¹Mitsubishi Tanabe Pharma Corporation, Kanagawa, Japan; ²Case Western Reserve University, Cleveland, OH; ³Protein Metrics, LLC, Cupertino, CA
- WP 291 **Nylon membrane immobilized acid protease digestion for hydrogen deuterium exchange capillary electrophoresis mass spectrometry;** Jordan Aerts¹; Per E. Andren¹; Erik T Jansson¹; ¹Uppsala University, Uppsala, Sweden
- WP 292 **Millisecond hydrogen/deuterium-exchange mass spectrometry of tryptophan side chains;** Jess Ramsay¹; Dr Daniel Kattinig¹; Dr Jonathan Phillips¹; ¹University of Exeter, Exeter, United Kingdom
- WP 293 **The Deuterium Calculator: A Python-based Tool for Bottom-up and Top-down Hydrogen-Deuterium Exchange Mass Spectrometry Data Analysis;** Kellye A Cupp-Sutton¹; Thomas Welborn¹; Mulin Fang¹; Joel Langford¹; Si Wu¹; ¹University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK
- WP 294 **Cross-Platform Standardization of Gas-Phase Hydrogen/Deuterium Exchange;** Alesi R Escobedo¹; Sunjit S. Uppal¹; Mike Guttman¹; ¹University of Washington, Seattle, WA
- WP 295 **New tools for aid with the analysis of bimodal HDX-MS data;** Miklos Guttman; ¹University of Washington, Seattle, WA
- WP 296 **Large Scale Investigation of Protein Stability and Dynamics Using High-Throughput Hydrogen-Deuterium Exchange Mass Spectrometry;** Allan J. R. Ferrari¹; Sugyan M Dixit¹; Jane M Thibeault¹; Gabriel J Rocklin¹; ¹Northwestern University, Chicago, IL
- WP 297 **HDX-MS with in-line electrochemical reduction of disulfide bonds – state of the art;** Hendrik-Jan Brouwer¹; Jean-Pierre Chervet¹; Martin Eysberg²; ¹Antec Scientific, Alphen a/d Rijn, Netherlands; ²Antec Scientific, Boston, MA 02108
- WP 298 **Operation at Constant Ultrahigh Resolution with 2wDetection using the Dynamically Harmonised Cell;** Benedict Gannon¹; Diana C Palacio Lozano¹; Hugh E Jones¹; Mark P. Barrow¹; ¹University of Warwick, Coventry, United Kingdom
- WP 299 **Handling the noticeable non-linearity of mass calibration in High resolution ToF MS;** Boris Kozlov¹; Sergey Kirillov²; ¹Waters, Wilmslow, United Kingdom; ²MSC-CG Ltd, Bar, Montenegro
- WP 300 **Increased sensitivity and throughput for native intact mass analysis using an online buffer exchange column;** Reiko Kiyonami¹; Weijing Liu¹; Rosa Viner¹; Min Du²; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, Boston, MA
- WP 301 **High Resolution mass spectrometry-based profiling of putative DNA adducts derived from trans,trans,2,4-decadienal (tt-DDE);** Yu-Ming Hsu¹; Chao-Yi Chen^{1, 2}; Tzu-Yu Pan¹; Acharee Kaewlaoyong¹; Min-Zong Huang¹; Chia-Fang Wu^{1, 2}; ¹Research Center for Precision Environmental Medicine, Kaohsiung Medical University, Kaohsiung city, Taiwan; ²International Master Program of Translational Medicine, National United University, Miaoli city, Taiwan

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- WP 302 **Comprehensive analysis of instrument parameters to achieve high-level ion focusing in linear time-of-flight mass spectrometry**; Yi-Hong Cai¹; Yi-Sheng Wang¹; ¹Genomics Research Center, Academia Sinica, Taipei, Taiwan
- WP 303 **Unlocking the potential of large-cohort proteomics studies with a novel high-resolution accurate mass platform**; Yue Xuan¹; Anna Pashkova¹; Martin Zeller¹; Colin Tobias Wirth¹; Jens Grote¹; Andreas Kuehn¹; Tabiwang N. Arrey¹; Eugen Damoc¹; Sally Webb²; Thomas Moehring¹; ¹Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ²Thermo Fisher Scientific, San Jose, CA
- WP 304 **Untargeted PFAS identification and targeted PFAS library screening workflows for groundwater analysis using a QTOF mass spectrometer**; Ethan R Hain¹; Kathleen Luo¹; Om Shrestha¹; Christopher Gilles¹; Evelyn Wang¹; Xiaomeng Xia¹; Robert English¹; Tiffany Liden¹; ¹Shimadzu Scientific Instruments, Columbia, MD
- WP 305 **A new approach for the comprehensive chemical description of complex pharmaceutical products via comprehensive gas chromatography and high-resolution mass spectrometry**; Ole Tiemann¹; Lukas Schwalb^{1,2}; Christopher Paul Rüger¹; Martha Liliana Chacón-patiño³; Thomas Gröger²; Ralf Zimmermann^{1,2}; ¹Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; ²Joint Mass Spectrometry Centre (JMASC), Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Zentrum München GmbH, German Research Center for Environmental Health, Neuherberg, Germany; ³National High Magnetic Field Laboratory, Tallahassee, FL
- WP 306 **Qualitative and quantitative analysis of Organic Solvents in lithium battery electrolysis by LC-QTOF**; Haiyang Wang¹; Zhihui Lin¹; Jianzhong Li²; Peibin Hu³; ¹Agilent Technologies, Inc, Guangdong, China; ²Agilent Technologies, Inc, Beijing, China; ³Agilent Technologies, Inc, Chengdu, China
- WP 307 **Determination of Oxytocin in the mouse brain by HR-UHPLC-MS: Method Development and Validation**; Hanin Diab¹; Jonathan Thompson²; Klementina Fon Tacer²; Tara Bayat²; ¹Texas Tech University, Amarillo, TX; ²School of Veterinary Medicine, Amarillo, Texas, United States, Amarillo, Texas
- WP 308 **A novel Ion Processor Device for High-Throughput Analysis in a High-Resolution Mass Analyzer**; Christian Hock¹; Hamish Stewart¹; Eduard Denisov¹; Amelia Peterson¹; Nicolaie Eugen Damoc¹; Martin Zeller¹; Tabiwang N. Arrey¹; Anna Pashkova¹; Alexander Wagner¹; Wilko Balschun¹; Alexander Kholomeev¹; Dmitry Grinfeld¹; Alexander A Makarov¹; ¹Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- WP 309 **Evaluation of Mass Correction Strategies for Accurate Mass Measurements of Pulsed Ionization Sources by Infrared Matrix-Assisted Laser Desorption Electrospray Ionization**; Alexandria L. Sohn¹; David C Muddiman¹; ¹North Carolina State University, Raleigh, NC
- WP 310 **Identification for Anions in Electrolyte of Lithium Battery Using Ion Chromatography - Quadrupole-Time of Flight Mass Spectrometry**; Zhihui Lin¹; Haiyang Wang¹; Jianzhong Li²; Peibin Hu³; ¹Agilent Technologies, Inc, Guangzhou, China; ²Agilent Technologies, Inc, Beijing, China; ³Agilent Technologies, Inc, Chengdu, China
- WP 311 **A Universal High-resolution Liquid Chromatography-Tandem Mass Spectrometry for the Analysis of N-nitrosodimethylamine in Pharmaceutical Products**; Donghee Lee¹; Se Hee Hong¹; Sang Beom Han¹; ¹Department of Pharmaceutical Analysis, College of Pharmacy, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul, South Korea
- WP 312 **Data Independent Analysis Evolution: Exploring the Use of High Resolving Power Multi-Reflecting Time-of-Flight Mass Spectrometry Selectivity for Metabolite Identification**; Michael McCullagh¹; Stephen Griffin²; Emma Marsden-Edwards¹; David Eatough¹; Dale Cooper-Shepherd¹; Martin Palmer¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters corp, milford, MA
- WP 313 **The Impact of ppb Mass Accuracy Upon Biotransformation Product Identification Using Negative Ion Non-targeted Urinary Screening Multi-Reflecting Time-of-Flight LCMS**; Michael McCullagh¹; Iggy Kass²; Emma Marsden-Edwards¹; David Eatough¹; Dale Cooper-Shepherd¹; Martin Palmer¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters, Milford, MA
- WP 314 **Thermal Analysis High-Resolution Mass Spectrometry in Material Sciences: Application towards Fiber-Reinforced Plastics/Concrete and their Thermal Stress and Recycling/Production Behavior**; Christopher Paul Rüger^{1,2}; Lukas Friederici¹; Anika Neumann¹; Arne Koch¹; Martha Liliana Chacón-patiño^{2,3}; Paolo Bomben⁴; Thorsten Streibel^{1,5}; Murray Gray^{4,6}; Ralf Zimmermann^{1,5}; ¹Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; ²International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harfleur, France; ³National High Magnetic Field Laboratory, Tallahassee, FL; ⁴Alberta Innovates, Calgary, AB; ⁵Joint Mass Spectrometry Center, Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, German Research Center for Environmental Health, Neuherberg, Germany; ⁶University of Alberta, Edmonton, AB
- WP 315 **Unveiling the performance of a novel high-resolution accurate mass platform for proteomics applications**; Tabiwang N. Arrey¹; Amirmansoor Hakimi²; Eduard Denisov¹; Nicolaie Eugen Damoc¹; ¹Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ²Thermo Fisher Scientific, San Jose, California
- WP 316 **Metabolomics and Lipidomics Profiling Applied to Bioprocessing using a Standardized, Quantitative Protocol with High-Resolution Mass Spectrometry**; Hoon Y Park¹; Stephen Dearth²; Hai Pham-Tuan²; Agnes Scharrer²; Vyncent Nguyen³; Didar Asik³; Chengjian Tu³; Ronny Dosanjh¹; John Point¹; George Bu¹; Elizabeth C Dodson¹; ¹Thermo Fisher Scientific, Hunt Valley, MD; ²Biocrates Life Sciences AG, Innsbruck, Austria; ³Thermo Fisher Scientific, Grand Island, NY
- WP 317 **Evaluation of a novel Tribrid Orbitrap Ascend system for in-depth high-throughput proteomics and phosphoproteomics**; Yuchen He¹; Katherine Overmyer^{1,2}; Dain R. Brademan^{1,2}; David Bergen³; Jingjing Huang³; Romain Huguet³; Michael W. Senko³; Vlad Zabrouskov³; Michael S. Westphall¹; Evgenia Shishkova¹; Graeme C McAlister³; Joshua J. Coon^{1,2}; ¹University of Wisconsin-Madison, Madison, WI; ²Morgridge Institute for Research, Madison, WI; ³ThermoFisher Scientific, San Jose, CA
- WP 318 **Enhanced ionization efficiency of astrobiologically relevant biomarkers via sample plate selection for Laser Desorption Ionization Mass Spectrometry (LDMS)**; Ashley M Hanna¹; Ziqin Ni²; Adrian Southard²; Ricardo Arevalo Jr.³; ¹University of Maryland, College Park, MD; ²University of Maryland College Park, College Park, MD; ³University of Maryland, College Park, College Park, MD
- WP 319 **Optimizing 7 Tesla FT-ICR MS equipped with frequency multiple detection and absorption mode processing for high throughput organic matter analysis**; Kevin J Zemaitis¹; Eric Choi¹; Rosalie Chu¹; Yuri E. Corilo¹; Sai Munikoti²; Jordan Rabus¹; Jan Strube²; William Kew¹; ¹Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; ²Pacific Northwest National Laboratory, Richland, WA

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- WP 320 **Urinary Forensic Toxicology Data Independent Analysis Screening: Using High Resolving Power Multi-Reflecting Time-of-Flight Mass Spectrometry;** Michael McCullagh¹; Johannes P.C. Vissers¹; Martin Palmer¹; Jane Cooper¹; Michelle Wood¹; Emma Marsden-Edwards¹; Nayan Mistry¹; ¹Waters Corporation, Wilmslow, United Kingdom
- WP 321 **New Tribrid MS ion optics and electronics improve sensitivity, duty cycle, and extend the MS range;** Graeme McAlister¹; Xiao Wang¹; Mike Goodwin¹; Christopher Mullen¹; Jesse D. Canterbury¹; Raman Mathur¹; Romain Huguet¹; David Bergen¹; Jingjing Huang¹; Michael W. Senko¹; Vlad Zabrouskov¹; ¹Thermo Fisher Scientific, San Jose, California
- WP 322 **Linking imaging mass spectrometry analysis of sepsis-induced metabolic rewiring and dichloroacetate treatment to septic cardiomyopathy;** Yu Tin Lin¹; Manal L. Zabalawi²; Lane M. Smith³; Peter W. Stacpoole⁴; Charles E. McCall²; Boone M. Prentice¹; ¹Department of Chemistry, University of Florida, Gainesville, FL; ²Department of Internal Medicine/Molecular Medicine and Department of Microbiology and Immunology, Wake Forest School of Medicine, Winston-Salem, NC; ³Department of Anesthesiology, University of Michigan Medical School, Ann Arbor, MI; ⁴Department of Medicine, Division of Endocrinology, Diabetes & Metabolism, and Department of Biochemistry and Molecular Biology, University of Florida College of Medicine, Gainesville, FL
- WP 323 **High resolution isomer resolved lipid imaging of the breast cancer tumor microenvironment;** Britt S.R. Claes¹; Annet A.M. Duivenvoorden¹; Caitlin M. Tressler²; Ethan Yang²; Kanchan Sonkar²; Shane R. Ellis^{1,3}; Kristine Glunde²; Ron M.a. Heeren¹; ¹Maastricht University, Maastricht, Netherlands; ²Johns Hopkins University School of Medicine, Baltimore, MD; ³University of Wollongong, Wollongong, Australia
- WP 324 **Quantification of cholesterol metabolites in the brain by on-tissue derivatization mass spectrometry imaging in a mouse model of Huntington's disease;** Alice Passoni¹; Angela Marika Siciliano¹; Monica Favagrossa¹; Alessia Lanno¹; Laura Colombo¹; Mario Salmona¹; Renzo Bagnati¹; Enrico Davoli¹; ¹Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy
- WP 325 **Mass spectrometry imaging and LC/MS/MS profiling of changes in host lipid metabolism of Mycobacterium tuberculosis infected MGL-1 deficient mice.;** Reina Paez¹; Sadhana Chauhan¹; Kubra F. Naqvi²; Janice Endsley¹; Brendan Prideaux¹; ¹University of Texas Medical Branch, Galveston, TX; ²University of Texas Southwestern Medical Center, Dallas, TX
- WP 326 **Discovery of Metabolite Biomarkers in Post-traumatic stress disorder (PTSD) Using Mass Spectrometry Imaging (MSI);** Huiying Guo¹; Shuli Tang¹; Jiaxin Feng¹; Luchen Wuyang¹; Xin Yan¹; ¹Texas A&M University, College Station, TX
- WP 327 **Spatial metabolomics identifies adenine as a new biomarker for pathology in patients with non-macroalbuminuric diabetic kidney disease;** Guanshi Zhang¹; Leila Hejazi^{1,2}; Petter Bjornstad³; Hak Joo Lee¹; Nerlyon Garcia Ponce De Leon¹; Christopher R. Anderton⁴; Theodore Alexandrov⁵; Manjeri A. Venkatachalam¹; Kumar Sharma¹; ¹UT Health San Antonio, San Antonio, TX; ²SyngnaMap, Inc., San Antonio, TX; ³University of Colorado Anschutz Medical Campus, Aurora, CO; ⁴Pacific Northwest National Laboratory, Richland, WA; ⁵European Molecular Biology Laboratory, Heidelberg, Germany
- WP 329 **Spatial Mapping of Lipids and Elements by Mass Microscopy and Integration with LA-ICP-MS in the Diabetic Mouse Pancreata;** Koji Okuda¹; Ei-ichi Matsuo¹; Jeffrey Dahl²; Toshiya Matsubara²; Shinichi Yamaguchi¹; Jannine I. Gamayot³; Shihwei Chen³; Christine M. Kusminski³; Philipp E. Scherer³; Ruth Gordillo³; ¹Shimadzu Corporation, Kyoto, Japan; ²Shimadzu Scientific Instrument, Columbia, Maryland; ³University of Texas Southwestern Medical Center, Dallas, TX
- WP 330 **Spatially resolved characterization of regulated molecules in host-parasite interactions using HR AP-SMALDI MSI;** Katja R Wiedemann¹; Stefanie Gerbig¹; Parviz Ghezellou¹; Nils H Anschütz¹; Alejandra Peter Ventura¹; Martin Roderfeld²; Elke Roeb²; Thomas Quack³; Christoph G Grevelding³; Liliana M R Silva³; Carlos R Hermosilla³; Anja Taubert³; Kerstin Strupat⁴; Bernhard Spengler¹; ¹Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, 35392 Giessen, Germany; ²Gastroenterology, Justus Liebig University Giessen, 35392 Giessen, Germany; ³Institute of Parasitology, Justus Liebig University Giessen, 35392 Giessen, Germany; ⁴Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- WP 331 **Revealing molecular alterations in glomeruli with various lesions using CODEX Multiplex Immunofluorescence and MALDI IMS;** Ellie L Pingry^{1,2}; Melissa A Farrow^{1,3}; Nathan Heath Patterson^{1,3}; Martin Dufresne^{1,3}; Jamie L Allen^{1,3}; Angela RS Kruse^{1,3}; Agnes B Fogo^{4,5,6}; Mark P Decaestecker^{2,4}; Jeffrey M Spraggins^{1,2,3,7}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Department of Nephrology, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; ⁵Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; ⁶Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; ⁷Department of Chemistry, Vanderbilt University, Nashville, TN
- WP 332 **MALDI HiPLEX-IHC on Tissue Microarrays in Neuropathology Research;** Yasemin Ucal¹; D.r. Naomi Vos¹; S. Alexandra Iakab¹; Henri Bogumil²; Rouzbeh Benan²; Gargey B. Yagnik³; Signe Frost Friedrichsen⁴; Corinna Henkel⁴; Mark Lim³; Andreas Von Deimling^{2,5}; Carsten Hopf^{1,6}; ¹Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim University of Applied Sciences, Mannheim, Germany; ²Department of Neuropathology, Institute of Pathology, Heidelberg University Hospital, Heidelberg, Germany; ³AmberGen, Inc., Billerica, MA; ⁴Bruker Daltonik GmbH, Bremen, Germany; ⁵Klinische Kooperationseinheit Neuropathologie, Deutsches Krebsforschungszentrum (DKFZ), Heidelberg, Germany; ⁶Medical Faculty, Heidelberg University, Heidelberg, Germany
- WP 333 **Imaging Mass Spectrometry Analysis of Gastric Proteome Changes after Helicobacter Pylori Infection in Gerbils;** Michelle L. Reyzer¹; Jennifer Shuman¹; Audra M. Judd¹; Hayes McDonald¹; Kevin L. Schey¹; Timothy L. Cover^{1,2}; Richard M Caprioli¹; ¹Vanderbilt University, Nashville, TN; ²Veterans Affairs Tennessee Valley Health Care System, Nashville, TN
- WP 334 **Multimodal Mass Spectrometry Imaging of Key Biomarkers To Study Ocular Disease;** Joshua J O Millar¹; Susan Campbell¹; Catherine Duckett¹; Sarah Doyle²; Laura Cole¹; ¹Sheffield Hallam University, Sheffield, United Kingdom; ²Trinity College Dublin, Dublin, Ireland
- WP 335 **Imaging of Fatty Acids in Brains Influenced by Cannabis and the Control of Unwanted Lipid Fragmentation;** Samantha L. Cousineau¹; Mohammed H. Sarikahya¹; Kristina Jurcic¹; Steven R. Laviolette¹; Ken K.-C. Yeung¹; ¹University of Western Ontario, London, ON
- WP 336 **Integrating label-free MALDI, MALDI HiPLEX-IHC and SepQuant mass spectrometry imaging to drive drug discovery and development;** Bingming Chen¹; Jarod Fincher¹; Mark Cancilla¹; ¹Merck, West Point, PA
- WP 337 **Enhancement of Lipid Signals in Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry with**

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- Ammonium Fluoride as a Matrix Additive;** Joseph H. Holbrook¹; Emily R. Sekera²; Arbil Lopez²; Brian D. Fries²; Fernando Tobias²; Kubra Akkaya³; Maria M. Mihaylova^{1,3,4}; Amanda B. Hummon^{1,2,4}; ¹The Ohio State University-Ohio State Biochemistry Program, Columbus, OH; ²The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; ³The Ohio State University-Department of Biological Chemistry and Pharmacology, Columbus, OH; ⁴The Ohio State University-Comprehensive Cancer Center, Columbus, OH
- WP 338 **Label-Free High-Resolution Molecular Imaging of Stratium Corneum by Cluster Secondary Ion Mass Spectrometry (Cluster SIMS);** Naoko Sano¹; Kate McHardy¹; Paul Blenkinsopp¹; ¹Ionoptika Ltd, Eastleigh, United Kingdom
- WP 339 **Multi-step workflow for visualisation of drug/metabolites and metabolism with DESI TQ and DESI Q-ToF mass spectrometers;** Emmanuelle Claude¹; Nyasha Munjoma¹; Alex Birsan²; Ian D Wilson³; Joanne B Ballantyne¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters Limited, Quebec, N/A; ³Division of Systems Medicine, Department of Metabolism Department of Metabolism, Digestion and Reproduction, Imperial College, Burlington Danes Building, Du Cane Road, London, United Kingdom
- WP 340 **Mass Spectrometry Profiling of N-Glycans in the Diabetic Pancreas;** Dylan Nicholas Tabang¹; Hua Zhang²; Daniel M. Tremmel^{3,4}; Sara Dutton Sackett³; Jon Odorico³; Lingjun Li^{1,2}; ¹Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ²School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ³Department of Surgery, University of Wisconsin-Madison, Madison, WI; ⁴Department of Surgery, Boston Children's Hospital, Boston, MA
- WP 341 **Improving spatial distribution sensitivity and selectivity in MSI, using a novel DESI-QqQ and HR-Multi Reflecting ToF systems;** Emmanuelle Claude¹; Farid Jahouh²; Martin E. Palmer¹; Inneke Wynant²; Filip Cuyckens²; Marjolein Van Heerden²; Jan Claereboudt³; Rob J Vreeken^{2,4}; Lance Nicolay⁵; ¹Waters Corporation, Wilmslow, United Kingdom; ²Preclinical Sciences & Translational Safety, Janssen R&D, Beerse, Belgium; ³Waters Corporation, Antwerpen, Belgium; ⁴Maastricht Multimodal Molecular Imaging Institute, Maastricht University, Maastricht, Netherlands; ⁵Waters Corporation, Milford, MA
- WP 342 **Targeted Quantitative Analysis of the Effect of Fomepizole on Acetaminophen Nephrotoxicity with a DESI Tandem Quadrupole MS Imaging Platform;** Jephthe Akakpo¹; Anthony Midey²; Bindesh Shrestha²; Hartmut Jaeschke¹; Anup Ramachandran¹; ¹University of Kansas Medical Center, Kansas City, KS; ²Waters Corporation, Milford, MA
- WP 343 **Mapping Physiologically Relevant Concentrations of Morphine in the Brain by IR-MALDESI MSI;** Yury Desyaterik¹; Austin M. Jones²; Kara M. Rademeyer²; Mary Peace McRae²; Angela D. M. Kashuba¹; Elias P. Rosen¹; ¹UNC, Chapel Hill, NC; ²Virginia Commonwealth University, Richmond, VA
- WP 344 **MALDI MSI visualizes the efficacy of cell therapy for treatment of mucopolysaccharidosis in murine brain;** Axel Treu¹; Panagiotis Douvaras²; Tim Brandenburger¹; Beate Schnippert¹; Diego F. Buenaventura²; Ashley Lepack²; Christoph Patsch²; Uwe Thuss¹; ¹Bayer AG, Wuppertal, Germany; ²BlueRock Therapeutics, New York City, NY
- WP 345 **Enhanced Detection of Brain Charged N-glycans by Infrared Matrix-Assisted Laser Desorption Electrospray Ionization Mass Spectrometric Imaging (IR-MALDESI-MSI);** Juhi Samal¹; Tana V. Palomino²; Judy Chen¹; David C Muddiman²; Tatiana Segura¹; ¹Duke University, Durham, NC; ²North Carolina State University, Raleigh, NC
- WP 346 **Glycosphingolipids are important for immune response in Schistosoma mansoni infected hamster liver - tissue studies with high resolution AP-SMALDI MSI;** David Luh¹; Sven Heiles^{1,2,3}; Martin Roderfeld⁴; Christoph G. Grevelding⁵; Elke Roeb⁴; Kerstin Strupat⁶; Bernhard Spengler¹; ¹Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, 35392 Giessen, Germany; ²Leibniz Institute for Analytical Sciences - ISAS - e.V., 44139 Dortmund, Germany; ³Lipidomics, Faculty of Chemistry, University of Duisburg-Essen, 45141 Essen, Germany; ⁴Gastroenterology, Justus Liebig University Giessen, 35392 Giessen, Germany; ⁵Institute for Parasitology, Justus Liebig University Giessen, 35392 Giessen, Germany; ⁶Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- WP 347 **Desorption electrospray ionization – mass spectrometry imaging using cyclic ion mobility improves for the separation of lipids isobars;** Ludovic Muller¹; Nivedita Hegdekar²; Chinmoy Sarkar³; Marta M. Lipinski³; Maureen A. Kane¹; ¹University of Maryland, School of Pharmacy, Baltimore, MD; ²University of Maryland, School of Medicine, Baltimore, MD; ³University of Maryland, School of Medicine, Baltimore, Maryland
- WP 348 **MALDI IMS Reproducibility for the Study of Large Sample Cohorts;** Katerina V Djambazova^{1,2}; Lukasz G Migas³; Martin Dufresne^{2,4}; Jamie L. Allen^{4,5}; Nathan Heath Patterson^{2,4}; Raf Van De Plas^{2,3,4}; Jeffrey M Spraggins^{1,2,4,6}; ¹Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; ²Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ³Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ⁴Vanderbilt University, Department of Biochemistry, Nashville, TN; ⁵Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ⁶Department of Chemistry, Vanderbilt University, Nashville, TN
- WP 349 **Mapping Alzheimer's disease with integrated MALDI IMS and highly multiplexed immunofluorescence microscopy;** Claire F Scott^{1,2,3}; Cody R Marshall^{2,3,4}; Wilber Romero Fernandez³; Melissa A Farrow^{2,3,6}; Angela Kruse^{2,3,6}; Allison B Esselman^{2,3,7}; Katerina V Djambazova^{1,2,3}; Martin Dufresne^{2,3,6}; Matthew S Schrag⁵; Jeffrey M Spraggins^{1,2,3,4,6,7}; ¹Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; ²Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ³Biomolecular Multimodal Imaging Center, Vanderbilt University, Nashville, TN; ⁴Chemical Physical Biology Program, Vanderbilt University School of Medicine, Nashville, TN; ⁵Department of Neurology, Vanderbilt University, Nashville, TN; ⁶Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁷Department of Chemistry, Vanderbilt University, Nashville, TN; ⁸Cerebral Amyloid Angiopathy Clinic, Vanderbilt University Medical Center, Nashville, TN
- WP 350 **Metabolite biomarkers associated to specific anatomical areas of a formalin-fixed paraffin embedded (FFPE) secondary lymphoid tissue;** Jeferson A. Valencia-Dávila¹; Benjamin L. Oyler¹; Richard Koupi¹; Constantinos Petrovas¹; ¹Tissue Analysis Core, Immunology Laboratory, Vaccine Research Center, NIAID, NIH, Bethesda, Maryland
- WP 351 **Mass spectrometry imaging of lipidome in a mouse model of blast-induced traumatic brain injury (TBI);** Mushfeqa Iqfath¹; Manxi Yang²; Palak Manchanda²; Julia Laskin²; Gaurav Chopra²; ¹Purdue University, West Lafayette, IN; ²Purdue University, WEST LAFAYETTE, IN
- WP 352 **Exploring in vivo deuterium labeling in surface tissues of Arabidopsis thaliana using MALDI-MS imaging;** Sumin Na¹; Young-Jin Lee¹; ¹Iowa State University, Ames
- WP 353 **Examining the Metabolic Factors Promoting Clostridioides difficile infection in Inflammatory Bowel Disease through Imaging Mass Spectrometry.;** Troy R. Scoggins¹; Amanda Pebenito^{2,3}; Jonathan T. Specker¹;

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- Joseph P. Zackular^{4,5}; Boone M. Prentice¹; ¹Department of Chemistry, University of Florida, Gainesville, FL; ²Division of Gastroenterology, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; ³Division of Protective Immunity, Children's Hospital of Philadelphia, Philadelphia, PA; ⁴Division of Protective Immunity, Children's Hospital of Philadelphia, Philadelphia, PA; ⁵Department of Pathology and Laboratory Medicine, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA
- WP 354 **Rapid and high spatial mapping of drugs by atmospheric pressure matrix-assisted laser desorption/ionization mass spectrometry imaging**; Ariful Islam¹; Md. Al Mamun¹; Muedur Rahman¹; Takumi Sakamoto¹; Tomohito Sato¹; Tomoaki Kahyo¹; Yutaka Takahashi¹; Mitsutoshi Setou¹; ¹Department of Cellular and Molecular Anatomy, Hamamatsu University School of Medicine, Hamamatsu, Japan
- WP 355 **Mass Spectrometry Imaging of Neurotransmitter Networks in DOX-Administered BRCA2 Knockout Mice Brains using FMP-10 Matrix**; Mathusha Pusparajah¹; Margi Patel¹; Berk U. Rasheed¹; Krishna K. Singh¹; Ken K.-C. Yeung¹; ¹Western University, London, ON
- WP 356 **Trace Level Quantification of Nitrosamine Impurities in Tuberculosis Medicines by LC-MS/MS**; Qi Yao Li¹; Qun Xu¹; Nadine Lo¹; Allan Leeks¹; Mark Han¹; Marcela Nefliu¹; Jack Simpson¹; Jennifer Belsky¹; ¹USP, Rockville, MD
- WP 357 **Native Datalake; enabling a Data Pipeline for Data Analysis with small to medium Native datasets**; Ryan P Marchand¹; Richard Chapman²; Neil Landers¹; ¹Waters corp, milford, MA; ²Waters Corporation, Milford, MA
- WP 359 **Identification of Unknown Compounds Observed in the Leachables Study of a Protein Drug by Liquid Chromatography High-Resolution Mass Spectrometry**; Jie Du¹; Tracy Zhou¹; Sven Hackbusch²; Kelly Broster³; ¹Genentech Inc., South San Francisco, CA; ²Thermo Fisher Scientific, San Jose, CA; ³Thermo Fisher Scientific, Hemel, United Kingdom
- WP 360 **Sequence confirmation and impurity characterization of therapeutic oligonucleotides – A quality by design approach**; Giovanni Calderisi¹; Patrik Plattner¹; Agron Selami¹; ¹Bachem AG, Bubendorf, Switzerland
- WP 361 **Enhanced screening for Active Pharmaceutical Ingredients (APIs) through the integration of a single quadrupole mass spectrometer**; Kathleen K Luo¹; Ethan R Hain¹; Om K Shrestha¹; Evelyn H Wang¹; Xiaomeng Xia¹; Robert English¹; Tiffany Liden¹; Christopher Gilles¹; ¹Shimadzu Scientific Instruments, Columbia, MD
- WP 362 **Quantitative Analysis of Azido Impurities in Five Sartan Drug Substances using a Triple Quadrupole Mass Spectrometer**; Kate (xiaomeng) Xia¹; Logan Miller¹; Evelyn H. Wang¹; Tairu Ogura¹; Yoshiyuki Okamura¹; ¹Shimadzu Scientific Instruments, Columbia, MD
- WP 363 **Novel Time-of-Flight Residual Gas Analyzer (TOF-RGA) for in situ Real-time Process Monitoring**; Lukas Hofer¹; Sébastien Gasc¹; ¹Spacetek Technology AG, Gümligen, Switzerland
- WP 364 **Method for non-destructively screening wine cork stoppers for 2,4,6-trichloroanisole below the perception threshold at a sampling speed of 2 seconds**; Luca Cappellin¹; Luigi Ciotti¹; Manuel Hutterli¹; Michael Groessl¹; ¹TOFWERK, Thun, Switzerland
- WP 365 **An Improved Method for Quantifying Glyphosate Impurity in Glyphosate API using LC/MS/MS via Standard Addition**; Chun-Ye Sun¹; Shao-Zhen Wang¹; ¹Agilent Technologies (China) Co., Ltd, Shanghai, China
- WP 366 **Chemical composition profiles of residues from in situ burning of fresh and weathered conventional and unconventional oils**; Ashish Sarker; Trent University, Peterborough, ON
- WP 367 **Identification and quantification of 25 crystallization solvents in support of pharmaceutical solid-form screening studies using a single SIFT-MS method**; Frank Tarczynski¹; Joanna Bis¹; Elliott Franco¹; Leslie Silva²; Vaughan Langford³; ¹Alcami Corporation, Morrisville, NC; ²Syft Technologies, Los Angeles, CA; ³Syft Technologies, Christchurch Central City, New Zealand
- WP 368 **Operating, maintaining, and troubleshooting the sensitivity and robustness of timsTOF platforms for proteomics studies**; Benoit Fatou¹; Conor Mullens¹; Elizabeth Gordon¹; Diego Assis¹; Alvaro Sebastian Vaca²; Michael Krawitzky²; Matt Willetts¹; ¹Bruker Scientific LLC, Billerica, MA; ²Bruker Scientific LLC, San Jose, CA
- WP 369 **Equipment and facility decontamination of b-lactams and other allergenic pharmaceutical products using Chlorine dioxide with LC/MS/MS monitoring**; Robert D. Voyksner¹; Paul Lorcheim²; ¹LCMS Limited, Durham, NC; ²ClorDiSys Solutions Inc., Branchburg, NJ
- WP 370 **Improving Precision and Accuracy of a LC-MS/MS Quantitation Method by Implementing Automation of Sample Extraction Procedures**; Junlong Shao; Pharmaron ABS, Germantown, MD
- WP 371 **Understanding K. phaffii (Pichia pastoris) Host Cell Protein Clearance via Flow-through Affinity in Biomanufacturing using Proteomics Approaches**; Taufika Islam Williams¹; Leonard B Collins¹; Sobhana Sripathi¹; Stefano Menegatti¹; ¹NCSU, Raleigh, NC
- WP 372 **PTM localization score MaxTopos for data-independent acquisition data in MaxQuant applied to phosphoproteomics provides accurate site localization**; Pelagia Kyriakidou¹; Shamil Urazbakhtin¹; Tanja Bange²; Maria Robles²; Juergen Cox¹; ¹Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Martinsried, Germany; ²Institute of Medical Psychology and Biomedical Center, Faculty of Medicine, Ludwig-Maximilians-University, München, Germany
- WP 373 **XGBoost-based peptide spectral library prediction integrated into MaxQuant for DDA and DIA data analysis**; Shamil Urazbakhtin¹; Favio Salinas-Soto¹; Pelagia Kyriakidou¹; Juan Luis Restrepo-Lopez¹; Juergen Cox¹; ¹Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Martinsried, Germany
- WP 374 **Mass++ ver.4 – An open-source MS data viewer with enhanced basic functions and easy implementation of external software**; Satoshi Tanaka^{1,2}; Masaki Murase²; Masaki Kato^{2,3}; Hiroyuki Yamamoto^{2,4}; Tsuyoshi Tabata^{2,5}; Maiko Kusano^{2,6}; Shin Kawano^{2,7}; Susumu Goto³; Yasushi Ishihama⁵; Akiyasu C. Yoshizawa^{2,5,7}; ¹Trans-IT Co., Ltd., Mibu-machi, Japan; ²Mass++ Users Group, Kyoto, Japan; ³Data Knowledge Organization Unit, RIKEN Information R&D and Strategy Headquarters, RIKEN, Wako, Japan; ⁴Human Metabolome Technologies, Inc., Tsuruoka, Japan; ⁵Grad. School of Pharma. Sci., Kyoto Univ., Kyoto, Japan; ⁶School of Medicine, Showa Univ., Shinagawa, Japan; ⁷Toyama Intl. Univ., Toyama, Japan; ⁸DBCLS, DS, ROIS, Kashiwa, Japan
- WP 375 **Fully automated and spectrum-centric processing of parallel reaction monitoring (PRM) data**; Daniel P. Zolq¹; Tobias Schmidt¹; Siegfried Gessulat¹; Florian Seefried¹; Samia Ben Fredj¹; Mathias Wilhelm²; Martin Heinrich Frejno¹; ¹MSAID GmbH, Garching b.München, Germany; ²Computational Mass Spectrometry, Technical University of Munich, Freising, Germany
- WP 376 **Tissue deconvolution using cell-type specific protein profiles: The whole is more than the sum of its parts**; Justus Zeinert¹; Bernhard Y Renard¹; Christoph N Schlaffner¹; ¹Data Analytics and Computational Statistics Group, Hasso Plattner Institute, University of Potsdam, Potsdam, Germany
- WP 377 **Aligning DIA Proteomics Data in Space: A Large-Scale Citizen Science Project**; Toon Calens^{1,2}; Tine Claeys^{1,2}; Sander Willems³; Maarten Dhaenens⁴; Lennart Martens^{1,2}; ¹VIB-UGent Center for Medical Biotechnology, Gent,

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- Belgium; ²Ghent University, Ghent, Belgium; ³Department of Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Martinsried, Germany; ⁴Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium
- WP 378 **midialD: a spectra-centric pipeline for the analysis of the midiaPASEF data;** Mateusz Krzysztof Lacki¹; Ute Distler¹; Michał Piotr Startek^{1,2}; David Teschner³; Sven Brehmer⁴; Jens Decker⁴; Thilo Schild⁵; Jonathan R Krieger⁶; Florian Krohs⁴; Oliver Raether⁴; Andreas Hildebrandt³; Stefan Tenzer⁶; ¹University Medical Center, Johannes Gutenberg University, Mainz, Germany; ²Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; ³Institute for Informatics, Johannes-Gutenberg University, Mainz, Germany; ⁴Bruker Daltonics GmbH & Co.KG, Bremen, Germany; ⁵University Medical Center of Mainz, Mainz, Germany; ⁶Bruker Ltd., Milton, ON
- WP 379 **dia-PASEF Tools: a shiny App for data visualization and exploration of dia-PASEF data;** Alvaro Sebastian Vaca¹; Christopher Adams¹; Matthew Willetts²; ¹Bruker Scientific LLC, San Jose, CA; ²Bruker Scientific, LLC, Billerica, MA
- WP 380 **Panorama Enhancements for System Suitability, Multi-Attribute Method, and Protein Coverage;** Josh Eckels¹; Wendy Innis¹; Ankur Juneja¹; Sweta Jewargikar¹; Nicholas Shulman²; Vagisha Sharma²; Michael J. MacCoss²; Brendan MacLean²; ¹LabKey, San Diego, CA; ²University of Washington, Seattle, WA
- WP 381 **A Protein Functional Map Learned from Pan-cancer Multi-Omics Data Enriches Somatic Mutations, Understudied Genes, and Cancer Hallmarks;** Zhiao Shi¹; Jonathan Lei¹; Bing Zhang¹; ¹Baylor College of Medicine, Houston, TX
- WP 382 **Finding Cancer Hallmarks Through Changes in mRNA/protein Relationships;** Jose Humberto Giraldez Chavez¹; Samuel H Payne¹; ¹Brigham Young University, Provo, UT
- WP 383 **Pan-cancer proteogenomics expands the landscape of therapeutic targets;** Jonathan T Lei¹; Sara R Savage¹; Xinpei Yi¹; Bo Wen¹; Hongwei Zhao²; Lauren K Somes¹; Paul W Shafer¹; Dou Yongchao¹; Zhiao Shi¹; Qiang Gao²; Valentina Hoyos¹; Bing Zhang¹; ¹Baylor College of Medicine, Houston, TX; ²Zhongshan Hospital, Fudan University, Shanghai, China
- WP 384 **Untangling the Connection between Caloric Restriction and Prolonged Survival in Non-human Primates through a Multi-omics Approach;** Salma Ibrahim Abouelhasan¹; Katherine A. Overmyer^{2,3}; Timothy W. Rhoads^{4,5}; Rozalyn M. Anderson^{4,5,6}; Joshua J. Coon^{2,3,7}; ¹University of Wisconsin-Madison, Madison, WI; ²Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI; ³Morgridge Institute for Research, Madison, WI; ⁴Department of Nutritional Sciences, University of Wisconsin-Madison, Madison, WI; ⁵Department of Medicine, University of Wisconsin-Madison, Madison, WI; ⁶Geriatric Research, Education, and Clinical Center, William S. Middleton Memorial Veterans Hospital, Madison, WI; ⁷Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- WP 385 **Multiomic analyses of COVID-19 samples to identify molecular signatures;** Baptiste Bauvin^{1,2}; Claudia Carpentier¹; Thibaud Godon^{1,2}; Maxime Deraspe¹; Jacques Corbeil^{1,2}; ¹Corbeil Laboratory, CRCHU de Quebec - Université Laval, Quebec, QC; ²GRAIL, Université Laval, Quebec, Quebec
- WP 386 **Systems proteomics reveals SARS-CoV-2 variants evolve convergent molecular strategies to remodel host signaling and protein complexes;** Mehdi Bouhaddou¹; Ann-Kathrin Reuschl²; Benjamin Polacco³; Lucy G Thorne²; Manisha Ummadi³; Chengjin Ye⁴; Luis Martinez-Sobrido⁴; Lisa Miorin⁵; Kris White⁵; Danielle L Swaney³; Adolfo Garcia-Sastre⁵; Clare Jolly⁶; Lorena Zuliani-Alvarez⁷; Greg Towers⁶; Nevan J Krogan³; ¹UCLA Mednet, Los Angeles, CA; ²University College London, London, United Kingdom; ³UCSF, San Francisco, CA; ⁴Texas Biomedical Research Institute, San Antonio, Texas; ⁵Icahn School of Medicine at Mount Sinai, New York, NY; ⁶University College London, London, United Kingdom; ⁷Novartis Institutes for Biomed.Research, Inc., Cambridge, MA
- WP 387 **A complete, modular, and flexible proteogenomic pipeline for peptide neoantigen discovery and verification;** Tyler Jubenville¹; James E. Johnson¹; Sue Rathe¹; Flavia Popescu¹; Kyle Richards¹; Suzanne Coleman¹; Reid Wagner¹; Fengchao Yu²; Alexey I. Nesvizhskii²; Subina Mehta¹; Pratik D Jagtap¹; David Largaespada¹; Timothy J. Griffin¹; ¹University of Minnesota, Minneapolis, MN; ²University of Michigan, Ann Arbor, MI
- WP 388 **MIcId: a MS-based Workflow for Fast and Accurate Microbe Identification, Antibiotic Resistance Protein Identification, and Biomass Estimation;** Gelio Alves¹; Aleksey Y Ogurtsov¹; Roger Karlsson²; Daniel Jaen-Luchoro²; Beatriz Piñeiro-Iglesias²; Francisco Salvà-Serra²; Björn Andersson²; Edward R B Moore²; Yi-Kuo Yu¹; ¹CBB NCBI NLM NIH, Bethesda, MD; ²University of Gothenburg, Gothenburg, Sweden
- WP 389 **Multi-omics data integration reveals clinical associated biomolecules in type 2 diabetes;** Xiaoyuan Zhou¹; Alexey Stukalov¹; Brittany Lee-McMullen¹; Shadi Ferdosi¹; Amir Alavi¹; Guhan Venkataraman¹; Harendra Guturu¹; Anna Halama²; Frank Schmidt²; Karsten Suhre²; Daniel Hornburg³; ¹Seer Inc., Redwood City, CA; ²Weill Cornell Medicine - Qatar, Education City, Qatar; ³Seer Inc, Redwood City, CA
- WP 390 **Leveraging the I.A.A Suite to Study the Impact of Drought in Sorghum and Setaria Through Metabolomics GWAS and RNA-Seq;** Allen Hubbard¹; Louis Connelly¹; Shrikaar Kambhampati²; Collin Luebbert¹; Hui Jiang¹; Jennifer Barrett¹; Madison Pope¹; Xiaoping Li¹; Ivan Baxter¹; ¹Donald Danforth Plant Science Center, Saint Louis, MO; ²Salk Institute for Biological Sciences, La Jolla, California
- WP 391 **LinkedOmicsKB: A web portal for pan-cancer proteogenomics data analysis;** Sara R Savage¹; Yuxing Liao¹; Yongchao Dou¹; Zhiao Shi¹; Xinpei Yi¹; Wen Jiang¹; Jonathan T Lei¹; Bing Zhang¹; ¹Baylor College of Medicine, Houston, Texas
- WP 392 **Accurate inference of kinase activity from human tumor phosphoproteomics data connects genetic aberrations to kinase targets;** Eric J Jaehnig¹; Koi Pham²; Zhiao Shi¹; Wen Jiang¹; Sara R Savage¹; Karsten Krug³; D. R. Mani²; Bing Zhang¹; ¹Baylor College of Medicine, Houston, Texas; ²Broad Institute of MIT and Harvard, Cambridge, MA; ³Frontier Medicines Corporation, Boston, MA
- WP 393 **Higher and higher N: SimpliFi data analysis for the masses now takes masses of samples;** Jim Palmer¹; John Wilson¹; ¹ProtiFi, LLC, Farmingdale, NY
- WP 395 **Multiomic Biomarkers in Livers of Streptozotocin-High Fat Diet Induced Non-Alcoholic Steatohepatitis (NASH) Mouse Model;** Ashok Panda¹; Gayathree Karthikkeyan¹; Daniel Domingo Fernández¹; Venkata H. V Boddada¹; Virendra Chine¹; Yogesh Aher¹; Kundan Kumar¹; Goutam Mondal¹; Indranil Mukhopadhyay¹; Biswapriya B. Misra¹; Joe Rokicki¹; Viswa Colluru¹; ¹Enveda Biosciences, Boulder, CO
- WP 396 **A Cloud-scalable Software Suite for Large-Scale Proteogenomics Data Analysis and Visualization;** Taylor Page¹; Harsharn Auluck¹; Margaret Donovan¹; Aaron S Gajadhar¹; Edwin Kwok¹; Yuandan Lou¹; Theo Platt¹; Serafim Batzoglou¹; ¹Seer, Inc., Redwood City, CA
- WP 397 **Novel tandem nano and capillary flow LCMS-based approach for facile 24/7 proteome profiling with near 100% MS;** Runsheng Zheng¹; Martin Rendl¹; Christopher

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- WP 398 **High-Resolution Separation of Bioisomers Using Ion Cloud Profiling Method;** Xiaoyu Zhou¹; Zhuofan Wang¹; Jingjin Fan¹; Zheng Ouyang¹; ¹Tsinghua University, Beijing, China
- WP 399 **The new type of electron impact mass spectrometer of ultra high resolution on the bases of multielectrode harmonized Kingdon trap;** Eugene (evgeny) Nikolaev¹; Oleg Kharybin¹; Gleb Vladimirov¹; Sergey Gorbatov¹; Anton Lioznov¹; Petr Borisovets¹; Alexander Semenov¹; ¹Skolkovo institute of science and technology, Moscow Region, Russian Federation
- WP 400 **Depth Profiling Study on Organic Monolayer by using Ar-GCIB and LDI-ToFMS;** Ji Young Baek¹; Chang Min Choi²; ¹Korea Basic Science Institute, Cheongju, South Korea; ²Korea Basic Science Institute, Cheongju, South Korea
- WP 401 **Probing the First Stages of Photoinitiated Polymerisation with an On-Line Photochemical Reactor Coupled Mass Spectrometer;** Oisín J Shiels¹; Maria Menti-Platten²; Brett Burns²; Paul Keller²; Philip J Barker²; Adam J Trevitt²; ¹University of Wollongong, Wollongong, Australia; ²University of Wollongong, School of Chemistry, Wollongong, Australia
- WP 402 **A novel high capacity ion trap to enhance duty cycle of time of flight mass spectrometer;** Masuyuki Sugiyama¹; Shun Kumano¹; Yuichiro Hashimoto²; Akihiro Nojima¹; ¹Research & Development Group, Hitachi Ltd., Kokubunji-Shi, Japan; ²Hitachi-HighTech Corporation, Hitachinaka-shi, Japan
- WP 403 **Characterization of a Novel PTR-TOFMS Instrument for Next Level Analysis of the Gas and Particle Phase;** Alfons Jordan¹; Christian Lindinger¹; Markus Müller¹; Tobias Reinecke¹; Markus Leiminger¹; Klaus Winkler¹; Lukas Märk¹; Todd Rogers²; Philipp Sulzer¹; ¹IONICON Analytik GmbH., Innsbruck, Austria; ²Trace VOC, Kennewick, WA
- WP 404 **An innovative prototype of mass spectrometry system based on a nano-opto-electromechanical (NOEMS) resonator sensor;** Wioletta Trzpił¹; Adrien Reynaud²; Louis Dartiguelongue³; Vaitson Cumaku³; Guillaume Jourdan¹; Sébastien Hentz⁴; Christophe Masselon³; Marc Sansa¹; ¹CEA-Leti, Université Grenoble Alpes, F-38000, Grenoble, France; ²Oberon Sciences, 300 avenue des papeteries, Villard-Bonnot, France, Villard-Bonnot, France; ³CEA, IRIG, Grenoble, France; ⁴CEA, LITEN, Grenoble, France
- WP 405 **Development and hybridization of orthogonal acceleration ToFMS and QIT-ToF-SIMS;** Jaeyoung Eo¹; Chang Min Choi²; ¹Korea Basic Science Institute, Daejeon, South Korea; ²Korea Basic Science Institute, Cheongju, South Korea
- WP 406 **A Study of the Improved Limitations of Bicubic Interpolation for both Field Analysis and Trajectory Calculations in SIMION;** Robert Jackson¹; Mark Osgood¹; ¹Ashwood Labs, LLC, Wilton, NH
- WP 407 **Characterization of a detection system with high sensitivity and dynamic range for a novel HRAM mass spectrometer;** Johannes Petzoldt¹; Toby Shanley¹; Wilko Balschun¹; Philipp Cochems¹; Bernd Hagedorn¹; Christian Hock¹; Barak Lavi²; Daniel Mourad¹; Maximilian Ochmann¹; Robert Ostermann¹; Semyon Shofman²; Hamish Stewart¹; Alexander Wagner¹; Amit Weingarten²; Alexander A Makarov¹; ¹Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ²El-Mul Technologies Ltd., Rehovot, Israel
- WP 408 **Versatile, long-lifetime, wide dynamic range detector for TOF applications;** Jonathan Garell¹; Amit Weingarten¹; Semyon Shofman¹; Alexander Kadyshevitch¹; ¹El-Mul Technologies, Rehovot, Israel
- WP 409 **Detection and accurate mass measurement of difficult to handle negatively charged compounds using Chemical Ionization MS (CIMS);** Alan T. Taylor¹; Colin L Mackay¹; ¹University of Edinburgh, Edinburgh, United Kingdom
- WP 410 **TENG for the Masses: A Low-cost Triboelectric Ion Source for Lipid Double Bond Localization and Other Nanoelectrospray Applications;** Carter Asef¹; Facundo Fernandez¹; ¹Georgia Institute of Technology, Atlanta, GA
- WP 411 **On-Paper Electrokinetic Separation and Stacking Coupled to Paper Spray MS for Sub-ppt Screening of Per-/polyfluoroalkyl substances (PFAS) in Tap Water;** Magnus P Rydberg¹; Nicholas Manicke¹; ¹Indiana University Purdue University Indianapolis, Indianapolis, IN
- WP 412 **Development and Evaluation of a Novel Accumulation Ion Source for Chemically Instable Compounds;** Joshua Rieger¹; Sanna Benter¹; Markus Langner¹; Niklas Pengemann¹; Philippe Rotgänger¹; Hendrik Kersten¹; Thorsten Benter¹; ¹University of Wuppertal, Wuppertal, Germany
- WP 413 **Localization of labile tyrosine sulfation using an alternative electron-based MS/MS approach in positive and negative ion modes;** Mark Lies¹; Haichuan Liu²; Takashi Baba³; Zoe Zhang²; Elliott Jones²; ¹Sciex, Brea, CA; ²SCIEX, Redwood city, CA; ³SCIEX, Concord, ON
- WP 414 **LIFDI technique coupled to Orbitrap Exploris MS;** Mathias Linden¹; Tobias P. Wörner²; Kerstin Strupat²; H. Bernhard Linden¹; ¹Linden CMS, Weyhe, Germany; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- WP 415 **Catalyst-free high yield post column online microdroplet derivatization for LC/MS Detection of depurinating DNA adducts;** Husam . I. S Kafeenah¹; Shu-Hui Chen¹; ¹National Cheng Kung University, Tainan, Taiwan
- WP 416 **Automated microfluidic open interface for direct coupling of solid-phase microextraction to mass spectrometry to facilitate rapid and high-throughput analysis;** Wei Zhou¹; Emir Nazdrajić¹; Janusz Pawliszyn¹; ¹University of Waterloo, Waterloo, ON
- WP 417 **Automating Minimally-Invasive Liquid Microjunction Sampling to Profile Large, Intact Objects;** Hannah Amy Lawther¹; G. Asher Newsome¹; ¹Smithsonian Museum Conservation Institute, Suitland, MD
- WP 418 **Characterization and comparison of theta-capillary and single-channel capillary tip generation for use in nano-electrospray ionization;** Jacob B Hatvany¹; Emma-Le Olsen¹; Elyssia S. Gallagher¹; ¹Baylor University, Waco, TX
- WP 419 **Development of a compact TLC sampler for MS and its applications;** Yiming Wang; Shimadzu Research Laboratory (Shanghai) Co.Ltd., Shanghai, China
- WP 420 **AMMOTRACe project: "Detection of Ammunition Compounds in Marine Systems using Membrane Inlet Laser-Photoionization Mass Spectrometry (PIMS)";** Christian Gehm¹; Carolin Schwarz²; Sven Ehlert³; Denis Starostin-Penner^{2,3}; Johannes Passig²; Dominic Kastner⁴; Christian Menhard⁴; Eric Achterberg⁵; Andreas Walte³; Ralf Zimmermann²; ¹Leibniz Institute for Baltic Sea Research, Rostock, Germany; ²Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; ³Photonion GmbH, Schwerin, Germany; ⁴InnoLas Laser GmbH, Krailing, Germany; ⁵GEOMAR Helmholtz Centre for Ocean Research Kiel, Kiel, Germany
- WP 421 **Effect of PEG-modification to capillary surfaces for analysis of carbohydrates and carbohydrate-containing molecules using nano-electrospray ionization-mass spectrometry;** Emma-Le P. Olsen¹; Jacob B. Hatvany¹; Chih-Chieh Hsieh²; Craig A. Aspinwall²; Elyssia S. Gallagher¹; ¹Baylor University, Waco, TX; ²University of Arizona, Tucson, Arizona

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- WP 422 **Electrochemically etched tapered-tip stainless-steel electrospray-ionization emitters**; Jordan T. Aerts¹; Per E. Andren¹; Erik T. Jansson¹; ¹*Uppsala University, Uppsala, Sweden*
- WP 423 **In-Situ Liquid Biopsy Combined with Native Surface Mass Spectrometry and Top-Down/Bottom-Up Proteomics**; Raul Villacob¹; Sarah C Beno¹; Neda Feizi Gilandeh¹; Touradj Solouki¹; ¹*Baylor University, Waco, TX*
- WP 424 **Direct Sampling and Ionization of E-Cigarette Aerosol**; Nicole C Auvil¹; Mark E Bier¹; ¹*Carnegie Mellon University, Pittsburgh, PA*
- WP 425 **Controlled synthesis of oligopeptides from simple amino acids in aqueous microdroplets by triboelectric nanogenerator nanoelectrospray mass spectrometry**; Ziad Mahmoud¹; Daniel D. Vallejo¹; Facundo M Fernandez¹; ¹*School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA*
- WP 426 **A NOVEL METHOD FOR THE SAMPLING OF NATIVE IONS FROM A DISTANT LOCATION**; Sanna Benter¹; Markus Langner¹; Niklas Pengemann¹; Hendrik Kersten¹; Thorsten Benter¹; ¹*University of Wuppertal, Wuppertal, Germany*
- WP 427 **In-tip microextraction enables fast profiling of phospholipid isomers in plasma by mass spectrometry**; Qiqian Zhang¹; Penglong Lian¹; Zheng Ouyang¹; Wenpeng Zhang¹; ¹*State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China*
- WP 428 **Deep Ultraviolet Laser Ablation and Capture for Off-line Mass Spectrometry**; Kadeem O Hayes¹; Blessing Egbejiogu¹; Neda Feizi Gilandeh²; Kelcey B. Hines¹; Touradj Solouki²; Kermit K. Murray¹; ¹*Louisiana State University, Baton Rouge, LA*; ²*Baylor University, Waco, TX*
- WP 429 **High-Throughput 'Dip-n-Sip' OPI-MS/MS sampling**; Nate Hoxie¹; Savannah Wood¹; Vijay Veerisetty¹; Anthony Garrison¹; Pranav Bende¹; John Janiszewski¹; Jonathan Shrimp¹; Colin Kelly¹; Meghav Verma¹; Charles Bonney¹; Sam Michael¹; Matthew Hall¹; Peter Kovarik²; Chang Liu²; Thomas R. Covey²; ¹*NIH/NCATS, Rockville, MD*; ²*SCIEX, Concord, ON*
- WP 430 **Developing a low-cost general-purpose correlative multipoint inlet for immediately accessible atmospheric pressure and vacuum ionization methods**; Charles N McEwen^{1,2}; Milan Pophristic¹; ¹*Research and Development, MSTM, LLC, Philadelphia, Pennsylvania*; ²*Saint Joseph's University, Philadelphia, PA, United States, Philadelphia, Pennsylvania*
- WP 431 **Construction and applications of a "plate-source" on API mass spectrometers: a robust, fast, and sensitive ionization method operating from AP**; Sarah Trimpin¹; Trine Halvorsen²; James Wager-Miller³; Ken Mackie³; Milan Pophristic⁴; Charles McEwen⁴; Ellen Inutan⁵; ¹*Wayne State University, Detroit, MI*; ²*Department of Pharmacy, University of Oslo, Oslo, Norway*; ³*Psychological and Brain Sciences Campus, IU Bloomington, Bloomington, IN*; ⁴*Department of Chemistry and Biochemistry, Saint Joseph's University, Philadelphia, Pennsylvania*; ⁵*Department of Chemistry, Mindanao State University-Iligan Institute of Technology, Iligan City, Philippines*
- WP 432 **Detection of plasma ions by coupling a high resolution TOF-MS at minimum distance to EUV-light focus point.**; Niklas Pengemann¹; Adelind Elshani²; Ismael Gisch²; Hendrik Kersten¹; Sascha Brose²; Carlo Holly²; Peter Gust¹; Thorsten Benter¹; ¹*University of Wuppertal, Wuppertal, Germany*; ²*RWTH Aachen University, Aachen, Germany*
- WP 433 **Structural characterization and identity confirmation of anthocyanins in plant extracts by direct injection ion mobility-mass spectrometry**; River Pachulicz¹; Long Yu²; Blagojce Jovceviski¹; Vincent Bulone^{1,2,3}; Tara L Pukala¹; ¹*University of Adelaide, Adelaide, Australia*; ²*Flinders University, Adelaide, Australia*; ³*AlbaNova University Centre, Stockholm, Sweden*
- WP 434 **Separation and Quantification of Fentanyl Isomers with Liquid Chromatography-Ion Mobility-Mass Spectrometry (LC-IM-MS)**; Ralph Aderorho¹; Christopher D. Chouinard¹; ¹*Clemson University, Clemson, SC*
- WP 435 **Differentiation of Regioisomers of Sulfobenzoic Acid by Traveling-wave Ion Mobility Mass Spectrometry (TW-IM-MS)**; Athula Attygalle¹; Jinxin Zhang¹; Meenu Kumar¹; Spencer Pinto¹; ¹*Stevens Institute of Technology, Hoboken, NJ*
- WP 436 **Ion mobility tandem mass spectrometry of chondroitin sulfate disaccharide domains in biglycan**; Mirela Sarbu¹; Raluca Ica¹; Edie Sharon²; David E. Clemmer²; Alina D. Zamfir^{1,3}; ¹*National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania*; ²*Indiana University Bloomington, Bloomington, IN*; ³*Department of Technical and Natural Sciences, "Aurel Vlaicu" University of Arad, Arad, Romania*
- WP 437 **Separation and sequencing of isomeric proteoforms of intact proteins with multiple post-translational modifications by top-down IMS-MS/MS**; Francis Berthias¹; Maša Babović¹; Nurgül Bilgin²; Jasmin Mecinovic²; Ole Nørregaard Jensen¹; ¹*Department of Biochemistry and Molecular Biology, VILLUM Center for Bioanalytical Sciences, University of Southern Denmark, Odense, Denmark*; ²*Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, Odense, Denmark*
- WP 438 **Development of Automated Online, High-Throughput Native Ion Mobility Mass Spectrometry Methodologies for Biotherapeutic Screening**; Brock R Juliano¹; Henry W Li¹; Anna G Anders¹; Zhuoer Xie²; Brandon T Ruotolo¹; ¹*University of Michigan, Ann Arbor, MI*; ²*Amgen, Inc., Thousand Oaks, CA*
- WP 439 **Analysis of Crown Ether-Alkali Metal Complexes Derived from Monomeric and Polydisperse Polymer Samples**; Hawkins Shepard¹; Jody C. May¹; David M Hercules¹; John A. McLean¹; ¹*Vanderbilt University, Nashville, TN*
- WP 440 **Detection and Characterization of Bacteria in Surface Water using LC-IM-MS/MS**; Kimberly Y Kartowikromo¹; Orobola E Olajide¹; Ahmed M Hamid¹; ¹*Auburn University, Auburn, AL*
- WP 441 **Characterization of Diabetes Biomarkers using High Resolution Ion Mobility – Mass Spectrometry**; Michael W Christopher¹; Daniel Debord²; Boone M. Prentice¹; Richard A. Yost¹; Timothy J. Garrett¹; ¹*University of Florida, Chemistry Department, Analytical Chemistry Division, Gainesville, FL*; ²*MOBILion Systems, Inc., Chadds Ford, PA*
- WP 442 **Improving confidence: Suspect-screening identification of per- and polyfluoroalkyl substances (PFAS) in abandoned eggs using ion mobility and time-of-flight mass spectrometry**; Zacheriah A Gernold¹; Joshua S. Wallace^{1,2}; Alicia Perez-Fuentetaja³; Diana Aga^{1,2}; ¹*University at Buffalo, Buffalo, NY*; ²*RENEW Institute, Buffalo, New York*; ³*Buffalo State, The State University of New York, Buffalo, New York*
- WP 443 **CCS-awarewide-scope target screening utilizing LC-TIMS-HRMS and a new heatedESI source–The answer to environmental and human biomonitoring challenges**; Konstantina S. Diamanti¹; Reza Aalizadeh¹; Dimitrios E. Damalas¹; Georgios O. Gkotsis¹; Bob Galvin²; Artem Filipenko³; Carsten Baessmann⁴; Nikolaos S. Thomaidis¹; ¹*National and Kapodistrian University of Athens, Athens, Greece*; ²*Bruker UK Ltd., Coventry, United Kingdom*; ³*Bruker Daltonics, Billerica, MA*; ⁴*Bruker Daltonics GmbH & Co. KG, Bremen, Germany*
- WP 444 **A facile method to generate DDA spectral libraries for DIA analysis provides comparable proteome coverage to a library-free approach**; Jessica Wohlfahrt¹; Emilee Mustor¹; Jennifer Guergues¹; Lindsey N Shaw¹; Stanley Stevens Jr. ¹; ¹*University of South Florida, Tampa, FL*

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- WP 445 **Peptide collision cross section of 22 post-translational modifications**; Andreas Will¹; Denys Oliinyk¹; Florian Meier-Rosar¹; ¹*Jena University Hospital, Jena, Germany*
- WP 446 **Comprehensive 4D workflow for targeted and untargeted screening of PFAS in organisms from different trophic levels utilizing LC-VIP HESI(-)-TIMS-QToF MS**; Georgios O. Gkotsis¹; Dimitrios E. Damalas¹; Maria-Christina Nika¹; Bob Galvin²; Carsten Baessmann³; Nikolaos S. Thomaidis¹; ¹*National and Kapodistrian University of Athens, Athens, Greece*; ²*Bruker UK Ltd., Coventry, United Kingdom*; ³*Bruker Daltonics GmbH & Co. KG, Bremen, Germany*
- WP 447 **Analysis of Polysorbates with a High Resolution Ion Mobility Platform Based on SLIM Technology**; Dustin Klein¹; Komal Kedia¹; Adam Sutton¹; Jon Degnore²; Daniel Debord²; Xuanwen Shawn Li¹; Hillary A. Schuessler¹; ¹*Merck & Co., West Point, PA*; ²*MOBILion Systems, Inc, Chadds Ford, PA*
- WP 448 **Unlocking new levels of structural information for proteins relevant to cultural heritage using native and top-down mass spectrometry**; Daniel D Vallejo¹; Vaclav Krupicka²; Aleksandra Popowich³; Julie Arslanoglu³; Caroline Tokarski²; Facundo M Fernandez¹; ¹*Georgia Institute of Technology, Atlanta, GA*; ²*Institute of Chemistry and Biology of Membrane and NanoObjects (CBMN), CNRS UMR 5248, Bordeaux Proteome, University of Bordeaux, Bordeaux, France*; ³*The Metropolitan Museum of Art, New York City, NY*
- WP 449 **Characterization of polyubiquitinated proteins using ion mobility-mass spectrometry (IM-MS) supplemented with the collisional activation of ions**; Elizaveta Shestoperova¹; Eric Strieter¹; ¹*University of Massachusetts Amherst, Amherst, MA*
- WP 450 **Native HRIM-MS Eliminates Chemical Noise and Enables Quaternary Structure Analysis of ALS-associated SOD1 Proteoforms**; Md Amin Hossain^{1,2}; Brandon C. Miller¹; Roman Manetsch¹; Jared R. Auclair¹; Jeffrey N. Agar¹; ¹*Northeastern University, Boston, MA*; ²*Harvard Medical School, Boston, MA*
- WP 451 **High Performance Ion Mobility Spectrometry for Pharma Cleaning Validation: Directspray for Real-Time Analysis vs Autosampler for High-Throughput Batch Sample Analysis**; Julia Kaszycki¹; Rory McCrimmon¹; Ching Wu¹; ¹*Excellims Corporation, Acton, MA*
- WP 452 **Prediction of ion mobilities using molecular dynamics based ion-neutral collisions in an open simulation framework (IDSIMF)**; Michelle Rajkovic¹; Maja Hammelrath¹; Walter Wissdorf¹; Thorsten Benter¹; ¹*University of Wuppertal, Wuppertal, Germany*
- WP 453 **Ion Clustering and Transformation Reactions during Transit in the HiKE-IMS: Comparing Measurement and Model**; Alexander Haack^{1,2}; Christoph Schaefer¹; Scott Hopkins²; Stefan Zimmermann¹; ¹*Leibniz University Hannover, Hannover, Germany*; ²*University of Waterloo, Waterloo, ON*
- WP 454 **Simulation of Ion Trajectories in Travelling Wave IMS with an Open Simulation Framework (IDSIMF)**; Maja Hammelrath¹; Michelle Rajkovic¹; Walter Wissdorf¹; Thorsten Benter¹; ¹*University of Wuppertal, Wuppertal, Germany*
- WP 455 **Cutting Corners with SLIM: New Rounded Turn Design Improves IM Resolution and Mobility Range of HRIM Analysis**; Liulin Deng¹; Adam Engelson¹; Miriam Fico¹; Daniel Debord¹; ¹*MOBILion Systems, Chadds Ford, PA*
- WP 456 **Deep Ultraviolet Laser Ablation Electrospray Ionization for Native Mass Spectrometry**; Kelcey B. Hines¹; Neda Gilandeh²; Raul Villacob²; Touradj Solouki²; Kermit K. Murray¹; ¹*Louisiana State University, Baton Rouge, LA*; ²*Baylor University, Waco, TX*
- WP 457 **Enabling High Accuracy Collision Cross Section Measurements using Cyclic Ion Mobility-Mass Spectrometry**; Devin M. Makey¹; Ryan Schroeder¹; Keith Richardson²; David Langridge²; Jakub Ujma²; Kevin Giles²; Brandon T. Ruotolo¹; ¹*University of Michigan, Ann Arbor, MI*; ²*Waters Corporation, Wilmslow, United Kingdom*
- WP 458 **Using Rigid Molecules to Probe Roles of Charge State, Charge Distribution, and Mass Distribution on Ion Mobility**; David V Dearden¹; Savannah R Porter¹; Jamir Shrestha^{1,2}; Tina Heravi^{1,3}; ¹*Brigham Young University, Provo, UT*; ²*Intel Corporation, Portland, OR*; ³*ARUP Laboratories, Salt Lake City, UT*
- WP 459 **Ramping up the Performance in SLIM: Traveling Waveform Gradients Enhance Mobility, Resolution, Range, and Throughput**; Leonard Rorrer¹; Ryan Clingman¹; Sidney Buttrill, Jr.²; Gordon A. Anderson³; Miriam Fico¹; Daniel Debord¹; ¹*MOBILion Systems, Inc., Chadds Ford, PA*; ²*Consultant, Palo Alto, CA*; ³*GAA Custom Electronics, LLC, Benton City, WA*
- WP 460 **Time-resolved tandem-trapped ion mobility spectrometry/mass spectrometry reveals cooperativity in the unfolding of native-like proteins**; Tyler C Cropley¹; Fanny C Liu¹; Mengqi Chai¹; Christian Bleiholder¹; ¹*Florida State University, Tallahassee, FL*
- WP 461 **Measuring the Conformational Ensemble of Caspase-9 using Ion Mobility-Mass Spectrometry and Collision-Induced Unfolding**; Trisha W. Brady¹; Stacey Nash¹; Kristalle G. Cruz¹; Ishan V. Soni¹; Jeanne A. Hardy¹; Richard W. Vachet¹; ¹*University of Massachusetts Amherst, Amherst, MA*
- WP 462 **Multi-faceted MS-Enabled Discovery, Characterization, and Localization of a Novel D-Amino Acid-Containing Neuropeptide in the American Lobster Nervous System**; Gaoyuan Lu¹; Wenxin Wu¹; Vu Ngoc Huong Tran¹; Hua Zhang¹; Min Ma¹; Zhijun Zhu¹; Shuling Xu¹; Lingjun Li¹; ¹*University of Wisconsin-Madison, Madison, WI*
- WP 463 **Labeling strategies for inducing mass distribution shifts in high-resolution cyclic ion mobility separations coupled to mass spectrometry**; David L. Williamson¹; Gabe Nagy¹; ¹*University of Utah, Salt Lake City, UT*
- WP 464 **Regulations of Many Solution Structures of Chymotrypsin Inhibitor 2 through ESI-IMS-MS Measurements**; Hua Pan¹; Shannon A. Raab¹; Lucas W. Henderson¹; Samantha R. Schrecke²; Arthur Laganowsky²; David H. Russell²; David E. Clemmer¹; ¹*Indiana University Bloomington, Bloomington, IN*; ²*Texas A&M University, College Station, TX*
- WP 465 **Characterization of Conformational Isomers of Proteins using Ion Mobility and Collision Induced Unfolding**; Michael L Moore¹; Stacey Nash¹; Richard W Vachet¹; ¹*University of Massachusetts Amherst, Amherst, MA*
- WP 466 **Determining the gas-phase stability of chloramphenicol acetyltransferase (CAT) and the effects of ligand binding**; Alexis N. Edwards¹; Anthony J. Blue¹; Michael S. Cordes¹; Jessica M. Conforti¹; Michael A. Trakselis¹; Elyssia S. Gallagher¹; ¹*Baylor University, Waco, TX*
- WP 467 **Composite Multidimensional Ion Mobility-Mass Spectrometry for Improved Differentiation of Stereochemical Modifications**; Xia Xu¹; Li Han¹; Zhen Zheng²; Rui Zhao¹; Lingjun Li³; Xueguang Shao¹; Gongyu Li¹; ¹*Nankai University, Tianjin, China*; ²*Tianjin Medical University, Tianjin, China*; ³*University of Wisconsin-Madison, Madison, WI*
- WP 468 **Ion Mobility and Collision Induced Unfolding Reveal Lipid Nanoparticle-Induced Changes in RNA Structure and Stability**; Anna G Anders¹; Brandon T Ruotolo¹; ¹*University of Michigan, Ann Arbor, MI*
- WP 469 **IMS-IMS on a Cyclic Ion Mobility Instrument Coupled to Variable Temperature Electrospray Ionization Elucidates Structural Landscapes of Tetrameric Proteins**; Edie M. Sharon¹; Lucas W. Henderson¹; Sarah M. O'Keefe¹; David E. Clemmer¹; ¹*Indiana University Bloomington, Bloomington, IN*
- WP 470 **Trapped ion mobility mass spectrometry in nucleic acid drug-discovery: revealing conformation-specific**

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- preferential binding to regulatory structures of the SARS-CoV-2 genome; Ghazaleh Yassaghi¹; Thomas Kenderdine¹; Jyotsna Kumar¹; Daniele Fabris¹; ¹University of Connecticut, Storrs, CT
- WP 471 **Structural Characterization of Isomeric Indium-Doped Octanuclear Iron-Oxo Clusters with Cubane Core using Ion Mobility Mass Spectrometry**; Solita Marie Wilson¹; Holly Bohlin¹; Susana Herrera²; Raphael Raptis²; Julia Laskin¹; ¹Purdue University, West Lafayette, IN; ²Florida International University, Miami, FL
- WP 472 **Correlating Conformation to Function of Disease-linked Labile Protein Surface Modifications Using Glycoform-resolved Quantitative Unfolding Mass Spectrometry**; Yifei Jia¹; Yamei Wang¹; Gongyu Li¹; ¹Nankai University, Tianjin, China
- WP 473 **Predicting Collisional Cross Section at Ultra-High Precision Using Comprehensive Physics and Translational-Rotational Energy Partitioning**; Christopher Harrilal¹; Sandilya V.B. Garimella²; Jaehun Chun²; Yehia M. Ibrahim²; Carlos Larriba-Andaluz³; Gregory K Schenter²; Richard D. Smith²; ¹Pacific Northwest National Lab, Richland, WA; ²Pacific Northwest National Laboratory, Richland, WA; ³Indiana University Purdue University Indianapolis, Indianapolis, IN
- WP 474 **IMS-MS Investigation of Protein Structure and Stability when Sprayed from Solutions with Different pH Values**; Kalina Siehl¹; Alexis N. Edwards¹; Elyssia S. Gallagher¹; ¹Baylor University, Waco, TX
- WP 475 **Characterizing Perfluorohexanesulfonic acid Isomers with Multi-Pass Cyclic Ion Mobility Mass Spectrometry Combined with Collision Cross Section and Retention Time Modeling**; Jonathan Antle¹; Sarah Dowd²; Diana Aga¹; ¹University at Buffalo, Buffalo, NY; ²Waters Corporation, Milford, MA
- WP 476 **Elucidation of denatured protein structures through Ion Mobility Spectrometry Mass Spectrometry by comparison to Gas Phase Ion Structures of homopolymers**; Leyan Hua¹; Gandhi D Viraj^{1,2}; Carlos Larriba Andaluz¹; ¹IUPUI, Indianapolis, IN; ²Purdue University, WEST LAFAYETTE, IN
- WP 477 **How good are the models proposed to rationalize the formation and transformation of gas-phase tautomeric ions**; Athula B. Attygalle; Stevens Institute of Technology, Hoboken, NJ
- WP 478 **Protein and Protein-DNA Thermal Conformational Changes studied by IR Laser-Assisted nESI-TIMS-ToF MS**; Samuel A Miller¹; Kevin Jeanne Dit Fouque¹; Fenfei Leng¹; Francisco Alberto Fernandez Lima¹; ¹Florida International University, Miami, FL
- WP 479 **Distinguishing Photo crosslinked and non-Photo crosslinked Human Telomers by Ion Mobility Mass Spectrometry**; Hsin-Chieh Yang¹; Savannah Scruggs¹; Mengqi Chai¹; John-Stephen Taylor¹; Michael L. Gross¹; ¹washington university in St. Louis, saint louis, MO
- WP 480 **Thermal Stabilities of Disulfide-Reduced Lysozyme Conformations by Cyclic Ion Mobility-Mass Spectrometry**; Sarah O'keefe¹; Lucas Henderson²; Edie M. Sharon²; David E. Clemmer³; ¹Indiana University, Bloomington, IN; ²Indiana University Bloomington, Bloomington, Indiana; ³Indiana University, bloomington, IN
- WP 481 **Conformation Identification of disaccharides by complexed with cyclodextrins and metal ions using ion mobility spectrometry and its application in foods**; Yinghua Yan¹; Chuan-Fan Ding²; ¹Ningbo University, Ningbo, China; ²Ningbo University, Ningbo, China
- WP 482 **Trapped ion mobility separation (tims) of glucose -6 phosphate and fructose 6 phosphate**; Surender Tadi¹; Xuejun Peng²; Beixi Wang³; Erica Forsberg⁴; Matthew Lewis⁵; ¹Bruker Daltonics, Billerica, MA; ²Bruker Scientific, San Jose, CA; ³Bruker Daltonics, San Jose, CA; ⁴Bruker Scientific, LLC, Billerica, MA; ⁵Bruker Dalton's GmbH & Co KG, Bremen, Germany
- WP 483 **Characterization of adeno-associated virus (AAV) capsid protein using microflow LC-MS/MS**; Lingsheng Chen¹; Tie Gao¹; Ji Luo²; Lihai Guo¹; Xiang Li³; Hongxu Chen¹; ¹SCIEX, Beijing, China; ²SCIEX, Shanghai, China; ³Division of Recombinant Biological Products, National Institutes for Food and Drug Control, Beijing, China
- WP 484 **Low level quantitation of seven N-nitrosamines in Monoclonal antibody (mAb) formulations by using LC-MS/MS**; Nitish Ramchandra Suryawanshi¹; Ashutosh Shelar¹; Deepti Maheshwari²; Samruddha Chavan¹; Nitin Shukla¹; Nilesh Patil¹; Purushottam Sutar¹; Dr. Jitendra Kelkar¹; Dr. Pratap Rasam¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; ²Spinco Biotech Pvt Ltd., Mumbai, India
- WP 485 **High-Throughput Quantification of Creatine Levels in Dried Blood Spot**; Keeley Jo Alexander¹; Fiona Hubbard²; Frances Morris²; Kavinda Desilva²; Mariko Nakano, PhD²; Charles Sailey, MEd; Zane Hauck, PhD²; ¹Molecular Testing Labs, Vancouver, WA; ²Molecular testing labs, Vancouver, WA
- WP 486 **Investigation of Ionization Mechanisms and Fragmentation Pathways of an Energetic Material Via Liquid Chromatography-High Resolution Mass Spectrometry (LC-MS)**; Kevin Pedersen¹; Elizabeth Grose¹; Andrew Horan¹; Ashly Huber¹; Joseph Worthington¹; Alicia Broderick²; John Brady²; ¹Signature Science, LLC, Egg Harbor Township, NJ; ²Transportation Security Laboratory, Atlantic City, NJ
- WP 487 **Ultra-fast LC-MS Analyses using Short 10 mm Columns**; Matthew James¹; Tony Edge¹; David Dunthorne¹; Mark Fever¹; Katie Lawlor^{2,3}; Lewis Couchman³; Keng Tiong Ng⁴; Leon Barron⁴; Geoff Faden⁵; ¹Avantor, Theale, United Kingdom; ²Department of Analytical, Environmental and Forensic Sciences, King's College London, London, United Kingdom; ³Analytical Services International, St. George's - University of London, London, United Kingdom; ⁴Environmental Research Group, School of Public Health, Imperial College London, London, United Kingdom; ⁵MAC-MOD Analytical Inc., Chadds Ford, PA
- WP 488 **Analysis and simultaneous quantitation of isoform-specific phosphoinositide 3-kinase (PI3K) inhibitors in mice plasma by LC-MS/MS and its application to pharmacokinetics**; Michelle L Spruill¹; Ritu Bohat²; Howard Martin³; Weiyi Peng²; Xinli Liu¹; ¹Department of Pharmacological and Pharmaceutical Sciences, University of Houston, Houston, TX; ²Department of Biology and Biochemistry, University of Houston, Houston, TX; ³Sagis Diagnostics, Houston, TX
- WP 489 **Microflow 4D-Proteomics for robust, high-throughput sample analysis**; Florian Busch¹; Andreas Schmidt¹; Johanna Tüshaus²; Eike Mucha¹; Thomas Kosinski¹; Stephanie Kaspar-Schoenefeld¹; Christoph Krisp¹; Christoph Gebhardt¹; Julie Munoz¹; Jean-Francois Greisch³; Axel Maibaum¹; Markus Lubeck¹; Bernhard Küster²; Gary Kruppa⁴; ¹Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ²Chair of Proteomics and Bioanalytics, TUM, Freising, Germany; ³Bruker Switzerland AG, Faellanden, Switzerland; ⁴Bruker S.R.O., Brno, Czech Republic
- WP 490 **Highly sensitive quantitation of N-nitroso-propranolol in Propranolol hydrochloride formulation and its placebo by using LC-MS/MS**; Nitin Shukla¹; Nitish Ramchandra Suryawanshi¹; Purushottam Sutar¹; Samruddha Chavan¹; Nilesh Patil¹; Dr. Jitendra Kelkar¹; Dr. Pratap Rasam¹; ¹Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India
- WP 491 **Optimization of search engines and data processing strategies using benchmark peptides enables highly sensitive and reliable MHC immunopeptidome analysis**; Sailee Rasam¹; Xiaoyu Zhu²; Timothy Sikorski³; Thomas Angel³; John T Mehl³; Jun Qu^{1,2}; ¹Department of

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- Biochemistry, State University of New York, Buffalo, NY; ²Department of Pharmaceutical Sciences, State University of New York, Buffalo, NY; ³GlaxoSmithKline, Collegeville, PA
- WP 492 **LC-MS determination of bleomycin in biological and pharmaceutical specimens;** Helena Plešnik^{1,2}; Maša Bošnjak^{3,4}; Maja Čemažar^{4,5}; Gregor Serša^{4,6}; Tina Kosjek^{1,2}; ¹International Postgraduate School Jožef Stefan, Ljubljana, Slovenia; ²Jožef Stefan Institute, Ljubljana, Slovenia; ³Faculty of Pharmacy, University of Ljubljana, Ljubljana, Slovenia; ⁴Department of Experimental Oncology, Institute of Oncology Ljubljana, Ljubljana, Slovenia; ⁵Faculty of Health Sciences, Izola, Slovenia; ⁶Faculty of Health Sciences, University of Ljubljana, Ljubljana, Slovenia
- WP 493 **Taking the characterization of bispecific antibodies with RPLC-MS to the next level by improving speed and selectivity;** Amarande Murisier¹; Valentina D'Atri¹; Vincent Larrailet²; Sebastian Pirner²; Miroslav Nikolov²; Davy Guillaume¹; ¹School of Pharmaceutical Sciences, Institute of Pharmaceutical Sciences of Western Switzerland, University of Geneva, Geneva, Switzerland; ²Roche Pharma Research and Early Development, Large Molecule Research, Penzberg, Germany
- WP 494 **It's All About the Solubility: Prodrug and Parent Bioanalysis Using LC-MS/MS;** Lin Bu¹; Woo Hyun Yoon¹; Danielle Tonev¹; Purvi Jejurkar¹; ¹Abbvie, South San Francisco, CA
- WP 495 **Analysis of Alkylphenol Ethoxylates (APEOs) and Alkylphenols (APs) in Textiles by UHPLC-MS/MS;** Jamie Foss¹; Francisco A. Ferron²; Roberto Bozic²; ¹PerkinElmer, Shelton, CT; ²PerkinElmer, Milan, Italy
- WP 496 **Global metabolic profiling of E. Coli strains for producing soluble recombinant protein;** Meghna Srivastava¹; Snehal Ganjave²; Deepti Sahastrabudhe²; Vivek Mishra³; Prajval Nakrani³; Pramod P. Wangikar^{2,3}; ¹Indian Institute of Technology, Bombay, Mumbai, India; ²Indian Institute of Technology Bombay, Mumbai, India; ³Clarity Bio Systems India Pvt Ltd, Pune, India
- WP 497 **Development of an analytical method by LC-HRMS for the analysis of saxitoxin and related Paralytic Shellfish Poisoning Toxins;** Salomé Chaumier¹; Clotilde Favino¹; Charlotte Mappa¹; Christine Albaret¹; Emmanuel Joubert¹; Anne Bossée¹; ¹DGA, Vert-Le-Petit, France
- WP 498 **Untargeted differential metabolomics of S. mutans biofilm on dental composites;** Chien-chia Chen¹; Karabi Mondal¹; Evan P. O'Brien¹; Karl J. Rockne¹; James L. Drummond¹; Luke Hanley¹; ¹University of Illinois at Chicago, Chicago, IL
- WP 499 **Characterization of a Diverse Sample Collection by UPLC-MS;** Wilfredo Pinto¹; Foster Tenkorang¹; ¹Merck, Rahway, NJ
- WP 500 **New Approach for Quantification and Measurement of Carbon Isotopes of Drugs with LC Coupled to FID and IRMS;** Herbert Tobias¹; Andrew Jones²; Tommy Saunders²; J. Thomas Brenna¹; ¹University of Texas at Austin, Austin, TX; ²Activated Research Company, Eden Prairie, MN
- WP 501 **Quantification of Psilocybin and Psilocin Content Variety in Psilocybe cubensis Strains with LC-MS;** Roman Goff¹; Morgan Smith¹; Jonathan Ferguson²; Kevin A. Schug¹; Sue Sisley³; Paige Wicker¹; ¹University of Texas at Arlington, Arlington, TX; ²Shimadzu Scientific Instrument, Columbia, MD; ³Scottsdale Research Institute, Scottsdale, AZ
- WP 502 **Development of an integrated and purpose-designed quality control workflow and dashboard for evaluation of LCMS proteomic platforms;** Lee K Palmer¹; Aaron O Bailey¹; William Russell¹; ¹University of Texas Medical Branch at Galveston, Galveston, TX
- WP 503 **Development and validation of a liquid chromatography-tandem mass spectrometry method for determination of phthalate and DINCH metabolites in human urine;** Zan Rekar^{1,2}; Agneta Annika Runkel¹; Darja Mazej¹; Tina Kosjek^{1,2}; Milena Horvat^{1,2}; ¹Department of Environmental Sciences, Jožef Stefan Institute, Ljubljana, Slovenia; ²International Postgraduate School Jožef Stefan, Ljubljana, Slovenia
- WP 504 **Direct Quantitation of Five Immunosuppressant Drugs in Volume-controlled Dried Whole Blood Spots by a Fully Automated DSM-LC-MS System;** Richard Gibson¹; Jingshu Guo¹; Stephanie N. Samra²; ¹Thermo Scientific, San Jose, CA; ²Thermo Scientific, San Jose, California
- WP 505 **Untargeted Mass Spectrometry for Analysis of Chemical Trends in Municipal Wastewater Before, During, and After the 2022 World Athletic Championships;** Sam Basset¹; Luke Marney²; Jeffrey Morre²; Thando Mawasha³; Michael Harry³; Casey Kanalos³; Corey De La Cruz⁴; Daphne Guo⁴; Cheng Shi⁴; Lya Carini⁴; Kyle Barber⁵; Gerrad Jones⁴; Christine Kelly³; Tyler Radniecki³; Claudia Maier^{2,6}; ¹Department of Biochemistry and Biophysics, Oregon State University, Corvallis, OR; ²Department of Chemistry, Oregon State University, Corvallis, OR; ³Chemical, Biological and Ecological Engineering, Oregon State University, Corvallis, OR; ⁴Department of Biological and Ecological Engineering, Oregon State University, Corvallis, OR; ⁵Athletics Integrity Unit, World Athletics, Monaco, Monaco; ⁶Linus Pauling Institute, Oregon State University, Corvallis, OR
- WP 506 **Maximizing Sensitivity by Multifactorial Optimization of Method Parameters for Clinical Mass Spectrometry;** Evan W. McConnell¹; Christopher M. Shuford¹; Russell P. Grant¹; ¹Labcorp, Burlington, NC
- WP 507 **Simultaneous detection and quantification of anticancer drug lapatinib, capecitabine, and 5-fluorouracil in blood and tissue by isotope dilution LC/MS/MS method;** Sana Sharif¹; Sujit Biswas¹; Michelle L Spruill¹; Xinli Liu¹; ¹University of Houston, Houston, TX
- WP 508 **Chiral LC-MS/MS Methods for the Direct Separation and Analysis of Enantiomers to Understand Conversion in vitro and in vivo;** Yongjin Yao¹; Bo Liu¹; Wenchen Luo¹; Cassandra Shu¹; Danielle Tonev¹; Purvi Jejurkar¹; ¹Abbvie, South San Francisco, CA
- WP 509 **Testosterone, Progesterone and Cortisol analysis by LC-MS/MS for Dried Blood Spot and Serum Samples in a 96-well preparation;** Joshua X Johnson; *Molecular testing labs, Vancouver, WA*
- WP 510 **The impact of posttranslational and chemical modifications on peptides retention in reversed-phase HPLC: a compendium of chromatographic data for proteomics;** Quinn Neale¹; Alexandre Prefontaine¹; Darien Yeung¹; Victor Spicer¹; Nediljko Budisa¹; Helene Perreault¹; Rene Zahedi¹; Oleg V. Krokhin¹; ¹University of Manitoba, Winnipeg, MB
- WP 511 **Structural characterization of SARS-CoV-2 dimeric ORF9b reveals potential fold switching trigger mechanism;** Xiyue Jin¹; Xue Sun²; Yan Chai³; Yu Bai³; Ying Li³; Tianjiao Hao³; Jianxun Qi³; Hao Song³; Catherine Ci Wong^{4,5,6}; George Fu Gao³; ¹University of Science and Technology of China, Hefei, China; ²Peking University, Beijing, China; ³Institute of Microbiology, Chinese Academy of Sciences, Beijing, China; ⁴Peking University, Beijing, China; ⁵Tsinghua-Peking University Joint Center for Life Sciences, Beijing, China; ⁶Peking Union Medical College Hospital, Beijing, China
- WP 512 **Direct analysis of in vitro oxidation of neural phospholipids via LC-MS/MS and GC-MS/MS;** Secilia Garza¹; Genevieve James¹; Hikyu Park¹; Paul Baker²; J. Thomas Brenna¹; ¹University of Texas, Austin, TX; ²SCIEX, Redwood city, CA
- WP 513 **Deep Profiling of Plasmalogens by Coupling the Paternò-Büchi Reactions with Tandem Mass Spectrometry;** Yichun Wang¹; Yu Xia¹; ¹Tsinghua University, Beijing, China
- WP 514 **Assessment of multiple separation dimensions for confident annotation of novel microbial conjugated bile**

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- acids (MCBAs) using ion mobility spectrometry-mass spectrometry;** James Dodds¹; Allison K Stewart²; Emily C Gentry³; Matthew H Foley⁴; Lee R Hagey⁵; Pieter C Dorrestein⁶; Casey M Theriot⁴; Erin S Baker¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC; ²Thermo Fisher Scientific, West Palm Beach, FL; ³Virginia Tech, Blacksburg, VA; ⁴North Carolina State University, Raleigh, NC; ⁵University of California San Diego, San Diego, CA
- WP 515 **A method for comprehensive investigation of lipid ligands using LC-FRC/HRMS/MS;** Noriyuki Tomiyasu¹; Yoshihiro Izumi²; Masatomo Takahashi²; Naoya Nishimura³; Kenji Toyonaga³; Sho Yamasaki³; Takeshi Bamba²; ¹Kyushu University, Fukuoka, Japan; ²Medical Institute of Bioregulation, Fukuoka, Japan; ³Research Institute for Microbial Diseases, Suita, Japan
- WP 516 **A charge-switching reagent for structure elucidation of branched-chain fatty acids via radical-directed dissociation;** Ruijun Jian¹; Yu Xia¹; ¹Tsinghua University, Beijing, China
- WP 517 **Enhanced Annotation of Low-Abundant Lipid Species using Experimentally Generated Libraries;** Nicholas S Ly¹; Jeremy K Chan¹; Cunjie Zhang¹; Andrew T Quail¹; Kelly Lozovschi¹; Stephanie Z Xie²; J. Rafael Montenegro-Burke¹; ¹Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON; ²Princess Margaret Cancer Centre, University Health Network, Toronto, ON
- WP 518 **Improving the performance of automated lipid identification for untargeted lipidomics;** William Xu¹; Adriana Zardini Buzatto¹; Elvis Lo¹; Shuang Zhao¹; Liang Li^{1,2}; ¹The Metabolomics Innovation Centre (TMIC), Edmonton, AB; ²University of Alberta, Edmonton, AB
- WP 519 **Comprehensive characterization of the lipid nanoparticle (LNP) ALC-0315 and its impurities using electron-activated dissociation (EAD);** Zhichang Yang¹; Sahana Mollah²; Paul Baker¹; Robert Proos³; Jon Le Huray⁴; ¹Sciex, Brea, CA; ²SCIEX, Redwood City, CA; ³Sciex, Framingham, MA; ⁴Acuitas Therapeutics Inc., Vancouver, BC
- WP 520 **Identifying Double-Bond-Positions of Phospholipids in Mouse Liver by Using Simultaneous Positive/Negative Ion Switching Analysis of LCMS-9050 and OAD-MS/MS;** Yohei Arao¹; Yuta Miyazaki¹; Hidenori Takahashi¹; ¹SHIMADZU Corporation, Kyoto, Japan
- WP 521 **The Caenorhabditis elegans lipidome blueprint – established using UHPLC-QTOF-MS and UHPLC-IMS-QTOF-MS;** Michael Tan¹; Liesa Salzer²; Aiko Barsch³; Sven W. Meyer³; Stefanie Wernisch³; Matthew R. Lewis³; Michael Wittig^{1,4}; ¹Metabolomics and Proteomics Core, Helmholtz Munich, Neuherberg, Germany; ²Research Unit Analytical BioGeoChemistry, Helmholtz Munich, Neuherberg, Germany; ³Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ⁴Chair of Analytical Foodchemistry, TUM School of Life Sciences, Technical University of Munich, Freising-Weihenstephan, Germany
- WP 522 **Understanding lipid metabolism in Type 1 Diabetes development using IMS-MS with ozone-induced dissociation and deep learning-based tool LipidOz;** Dylan H. Ross¹; Soumyadeep Sarkar¹; Aivett Bilbao¹; Joon-Yong Lee¹; Daniel J Orton¹; Josie G. Eder¹; Meagan C. Burnet¹; Richard D. Smith¹; Jennifer E. Kyle¹; Ernesto S. Nakayasu¹; Xueyun Zheng¹; ¹Pacific Northwest National Laboratory, Richland, WA
- WP 523 **Profiling double bond location of unsaturated lipids in human plasma with Total Correlation Mass Spectrometry (TOC-MS);** Jack Rice¹; Svitlana Liashenko¹; Nathan Cassidy¹; Peter B. O'Connor^{1,2}; ¹Verdel Instruments Ltd, Camberley, United Kingdom; ²University of Warwick, Coventry, United Kingdom
- WP 524 **The complexity of methyl-branched unsaturated fatty acids in the skin lipidome of newborns;** Lukáš Cudlman^{1,2}; Jan Philipp Menzel³; Monica Liu³; Prabhu Rangabashyam³; Venkateswara R Narreddula³; Stephen J Blanksby³; Josef Cvačka^{1,2}; ¹Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic; ²Department of Analytical Chemistry, Faculty of Science, Charles University, Prague, Czech Republic; ³School of Chemistry and Physics, Queensland University of Technology, Brisbane, Australia
- WP 525 **Gas-Phase Ion/Ion Strategy for the Differentiation of Isomeric Bis(monoacylglycerol)phosphate and Phosphatidylglycerol Species by Shotgun Lipidomics;** De'shovan M. Shenault¹; Caitlin E. Randolph¹; Sarah T. Nsiah¹; Scott A. McLuckey¹; ¹Purdue University, Lafayette, IN
- WP 526 **Tracking the metabolism of unsaturated fatty acids in Staphylococcus aureus using online Paternó-Büchi reactions;** Emily L Pruitt¹; Libin Xu¹; ¹University of Washington, Seattle, WA
- WP 527 **High-Energy Collision-Induced Dissociation and In-source Decay MALDI of Metal-adducted Fatty acids;** Chioma J Akor; ¹The University of Alabama, Tuscaloosa, AL
- WP 528 **Lipid Nanoparticle Impurity Monitoring Using Single Quadrupole Mass Detection for Regulated Environments;** Duanduan Han¹; Kellen Delaney¹; Robert E. Birdsall¹; Ying Qing Yu¹; ¹Waters Corporation, Milford, MA
- WP 529 **The atlas of brain glycosphingolipids revealed by selective enrichment and structural lipidotyping;** Zidan Wang¹; Donghui Zhang²; Wenpeng Zhang²; Yu Xia²; ¹Tsinghua university, Beijing, China; ²Tsinghua University, Beijing, China
- WP 530 **Identification and Characterization of Impurities in Lipid Nanoparticle Components Using TOF-MS with In-silico Fragmentation Data Processing;** Kellen Delaney¹; Duanduan Han¹; Robert E. Birdsall¹; Ying Qing Yu¹; ¹Waters Corporation, Milford, MA
- WP 531 **Determining Double Bond Positions of Lipids using Supercritical Fluid Chromatography Photoionization Mass Spectrometry and Collision-Induced Dissociation of Radical Cations;** Patrick Mueller¹; Gérard Hopfgartner¹; ¹University of Geneva, Geneva, Switzerland
- WP 532 **Resolve gut bacterial lipid isomerism by coupling mCPBA epoxidation with RPLC-MS/MS;** Kai-Li Chen¹; Ting-Hao Kuo¹; Cheng-Chih Hsu¹; ¹Department of chemistry, National Taiwan University, Taipei, Taiwan
- WP 533 **Localization of Methyl branching and Unsaturated Sites on Fatty Acids and Ganglioside with Radical-Initiated Dissociation via Charge-Switch Chemistry and LC/MS;** Shane M Finn¹; Wilton Gilles¹; Rayan Murtada¹; Jinshan Gao¹; ¹Montclair State University, Montclair, NJ
- WP 534 **Improved Separation of Lipid Extracts Using High Resolution Ion Mobility Incorporating Structures for Lossless Ion Manipulation in LC-HRIM-HRMS;** Allison R. Reardon¹; Katrina L. Leaptrot¹; Jody C. May¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN
- WP 535 **Structural diversity of Leptospira lipid A: what can it reveal about pathogenesis?;** Helena Petrosova^{1,2}; Abanoub Mikhael²; Matthew Sherman³; Sophie Culos¹; Alexandre Giraud-Gatineau⁴; Alloysius M. Gomez¹; Robert K Ernst³; Caroline E. Cameron^{1,5}; Elsie A. Wunder Jr.⁶; Mathieu Picardeau⁴; David R Goodlett^{1,2}; ¹University of Victoria, Victoria, BC; ²University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; ³University of Maryland, Baltimore, MD; ⁴Institut Pasteur, Paris, France; ⁵University of Washington, Seattle, WA; ⁶Yale School of Public Health, New Haven, CT
- WP 536 **Ozone-enabled fatty acid discovery reveals unexpected diversity in the human lipidome;** Jan Philipp Menzel¹; Reuben S. E. Young²; Aurelie H. Benfield³; Julia S. Scott^{4,5}; Puttandon Wongsomboon¹; Lukáš Cudlman^{6,7}; Josef Cvačka^{6,7}; Lisa M. Butler^{4,5}; Sonia T. Henriques³; Berwyck Poad¹; Stephen J Blanksby¹; ¹School of Chemistry and Physics, Queensland University of Technology, Brisbane, Australia; ²University of Wollongong, Wollongong, Australia;

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- ³*School of Biomedical Sciences, Faculty of Health, Queensland University of Technology, Translational Research Institute, Brisbane, Australia;* ⁴*South Australian Immunogenomics Cancer Institute and Freemasons Centre for Male Health and Wellbeing, University of Adelaide, Adelaide, Australia;* ⁵*South Australian Health and Medical Research Institute, Adelaide, Australia;* ⁶*Department of Analytical Chemistry, Faculty of Science, Charles University, Prague, Czech Republic;* ⁷*Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic*
- WP 537 **A comparative study on the identification of plasma lipids using collision-induced dissociation and electron-activated dissociation;** Kiran Maan¹; Dipankar Malakar¹; Cagakan Ozbalcı²; ¹SCIEX, Bangalore, India; ²SCIEX, Alderley Park, United Kingdom
- WP 538 **Detection and Characterization of Intact Oxidized Phospholipids Following Oxidative Insult of Immortalized Microglial Cells;** Yulemni Morel¹; Nivedita Hegdekar²; Chinmoy Sarkar²; Marta Lipinski²; Jace W Jones¹; ¹University of Maryland, Baltimore School of Pharmacy, Baltimore, MD; ²University of Maryland, Baltimore School of Medicine, Baltimore, Maryland
- WP 539 **Pathogenic Leptospira lipid A structural changes induced by growth conditions;** Sophie Culos¹; Helena Petrosova^{1,2}; Abanoub Mikhael¹; Alexandre Giraud-Gatineau³; Elsie A. Wunder Jr.⁴; Mathieu Picardeau³; David R Goodlett^{1,2}; ¹UVic Genome BC Proteomics Centre, Victoria, BC; ²Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; ³Biology of Spirochetes Unit, Institut Pasteur, Paris, France; ⁴Department of Epidemiology of Microbial Diseases, Yale School of Public Health, New Haven, CT
- WP 540 **Enhance lipid isomer analysis by online photochemical derivatization with capillary electrophoresis-mass spectrometry;** Junhan Wu¹; Yikun Liu¹; Wenpeng Zhang¹; Zheng Ouyang¹; ¹Tsinghua University, Beijing, China
- WP 541 **Structure-centric annotation of phospholipids by Electron Activated Dissociation;** Vincen Wu¹; Mario Povoia Correia¹; Adriano Rutz¹; Nicola Zamboni¹; ¹ETH Zurich, Zurich, Switzerland
- WP 542 **Activated Electron Photodetachment and Ultraviolet Photodissociation for Top-Down Characterization of Intact Bacterial Lipooligosaccharides;** James E Keener¹; Jennifer S Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- WP 543 **Lipidomic Profiling of Patients and Long-Term Survivors with Pancreatic Ductal Adenocarcinoma Using Reversed-Phase UHPLC/MS;** Zuzana Vaňková¹; Ondřej Peterka¹; Jakub Idkowiak¹; Robert Jirásko¹; Beatrice Mohelníková Duchoňová²; Martin Loveček²; Bohuslav Melichar²; Michal Holčapek¹; ¹University of Pardubice, Pardubice, Czech Republic; ²University Hospital Olomouc, Olomouc, Czech Republic
- WP 544 **High-coverage targeted lipidomics analysis by LC-MS/MS in mouse brain tissue prepared by laser-capture microdissection;** Chenchun Zhong; *SCIEX, Shanghai, China*
- WP 545 **Identification and quantification of unsaturated fatty acids using electron-activated dissociation (EAD) fragmentation;** Zhuo Man¹; Dandan Si²; Zhimin Long²; ¹sciex, beijing, China; ²SCIEX, Beijing, China
- WP 546 **Comparison of Plasma Triacylglycerols and Cholesteryl Esters Measured via Supercritical Fluid Chromatography and Normal Phase LC-MS/MS;** Eunice A Grigorutsa¹; Michael S Gardner¹; Susan Kuklennyk¹; John R Barr¹; ¹Centers for Disease Control and Prevention, Chamblee, GA
- WP 547 **Aziridination-Based¹³C-Isotope Labeled Tag for Lipid Accurate Relative Quantitation at the Isomer Level;** Hongyuan Yang¹; Shuli Tang¹; Syuan-Ting Kuo¹; Xin Yan¹; ¹Texas A&M Chemistry, College Station, TX
- WP 548 **An LC-MS/MS Method for Measurement of Sphingolipids in the Plasma of Pediatric Patients with Disorders of Sphingolipid Metabolism;** Joanna Y. Lee¹; Julie D. Saba¹; Hui Zhao²; Yanan Yang²; ¹Department of Pediatrics, Division of Hematology/Oncology, University of California-San Francisco, Oakland, CA; ²Agilent Technologies, Santa Clara, CA
- WP 549 **A C30 RP-LC-MS/MS method for the determination of cholesterol esters from fed and fasted human plasma and cells;** Trevor B Romsdahl¹; Jennifer J Linares¹; William K Russell¹; ¹Mass Spectrometry Facility - University of Texas Medical Branch, Galveston, TX
- WP 550 **Method for analyzing lipids and vitamins in media using HPLC-MS and GC-MS;** Hee-Jin Yoo¹; Duck-Hyun Kim²; Moonhee Park²; Kun Cho¹; ¹Korea Basic Science Institute, Ochang, South Korea; ²Korea Basic Science Institute, Ochang, South Korea
- WP 551 **Development and Analytical Validation of a Sphingolipid Targeted Panel;** Crystal L. Pace¹; Bradley C. Cochran¹; Richard J. Robinson¹; ¹Metabolon, Morrisville, NC
- WP 552 **Robust UPLC-MRM-MS workflow that allows combined quantification of oxylipins and PUFAs in a single analysis;** Mona Khorani¹; Liping Yang¹; Jaewoo Choi^{1,2}; Lynne H. Shinto³; Claudia S. Maier^{1,2}; ¹Department of Chemistry, Oregon State University, Corvallis, OR; ²Linus Pauling Institute, Oregon State University, Corvallis, OR; ³Department of Neurology, Oregon Health & Science University, Portland, Oregon
- WP 553 **Alterations of Brain Bioactive Lipids after Microglia Elimination in Alzheimer's Disease: A Functional Lipidomics Study;** Ziyang Xu¹; Juan Pablo Palavisini^{1,2}; Sepideh Kiani Shabestari^{3,4}; Mathew Blurton-Jones^{3,4,5}; Kevin F Bieniek⁶; Xianlin Han^{1,2}; ¹Barshop Institute for Longevity and Aging Studies, University of Texas Health Science Center at San Antonio, San Antonio, Texas; ²Department of Medicine, UT Health San Antonio, San Antonio, Texas; ³Department of Neurobiology & Behavior, UC Irvine, Irvine, California; ⁴Sue and Bill Gross Stem Cell Research Center, UC Irvine, Irvine, California; ⁵Institute for Memory Impairments and Neurological Disorders, UC Irvine, Irvine, California; ⁶Department of Pathology, Glenn Biggs Institute for Alzheimer's and Neurodegenerative Diseases, UT Health San Antonio, San Antonio, Texas
- WP 554 **Dual Cyclization tandem mass for quantification of phosphatidylcholines using 6-plex isobaric tagging;** Mahmoud Elhusseiny Mostafa¹; Julius Agongo¹; Reagan McGuffee¹; Scott Grady¹; Christopher Arnatt¹; David Ford¹; James Edwards¹; ¹Saint Louis University, Saint Louis, MO
- WP 555 **UPC2-MS/MS for Quantitation of a Panel of Polyunsaturated Fatty Acids and their Eicosanoid Oxylipin Metabolites;** Guille Metzler¹; Carmen Fernandez-Metzler¹; Richard C. King¹; ¹PharmaCadence Analytical Services, Hatfield, PA
- WP 556 **Lipid Mass Tags via Aziridination for Probing Unsaturated Lipid Isomers and Accurate Relative Quantification;** Tingyuan Yang¹; Shuli Tang¹; Syuan-Ting Kuo¹; Dallas Freitas¹; Madison Edwards¹; Hongying Wang¹; Yuxiang Sun¹; Xin Yan¹; ¹Texas A&M University, College Station, TX
- WP 557 **Targeted 4D PASEF-based quantification strategy for clinical lipidomics;** Dhanwin Baker¹; Raissa Lerner²; Laura Bindila²; ¹University Medical Center of Mainz, Mainz, Germany; ²University Medical Center of Mainz, Mainz, Germany
- WP 558 **Phytosterols profiling in human serum using a liquid chromatography tandem mass spectrometry;** Kersti Karu; *UCL Chemistry Mass Spectrometry Facility, London, United Kingdom*
- WP 559 **A targeted LC-MS method for identification and quantification of 10 different classes of phospholipids;** Rohit B. Kamble¹; Qibin Zhang^{1,2}; ¹Center for Translational

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- Biomedical Research, University of North Carolina at Greensboro, North Carolina Research Campus, Kannapolis, NC; ²Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, NC
- WP 560 **A derivatization strategy using isotopically-labeled 3-NPH for absolute quantitation of free fatty acids from human plasma by LC-MS/MS;** Jennifer J Linares¹; Trevor Romsdahl¹; William Russell¹; ¹UTMB Health Mass Spectrometry Facility, Galveston, TX
- WP 561 **An automated LC-PB-MS workflow for large-scale analysis of lipid C=C isomers;** Nan Zhang¹; Wenhui Pang¹; Jiexun Bu¹; Wenpeng Zhang²; Zheng Ouyang²; ¹PURSPEC Technology (Beijing) Ltd., Beijing, China; ²Tsinghua University, Beijing, China
- WP 562 **Direct Comparison of Targeted Ganglioside Analysis Using Multiple Reaction Monitoring (MRM) and Parallel Reaction Monitoring (PRM) LC-MS/MS;** Arvin Saffarian Delkosh¹; Akeem Sanni¹; Judith Nwaiwu¹; Andrew I. Bennett¹; Cristian D. Gutierrez-Reyes¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, Texas
- WP 563 **Paternò-Büchi (PB) reaction-based isobaric mass tags for accurate relative quantitation of fatty acids at the isomer level;** Xi Chen¹; Gopal Reddy Ramidi¹; Syuan-Ting Kuo¹; Dallas Freitas¹; Luchen Wuyang¹; Aidan Slagter¹; Peiyu Cai¹; Ashok Polu¹; Xin Yan¹; ¹Texas A&M University, College Station, TX
- WP 564 **Targeted Lipidomic Analysis of Pediatric Leukemia Cells Using LC-MS/MS Triple Quadrupole;** Lihua Jiang¹; Ruiqi Jian¹; Tiffany Trinh¹; Hui Zhao²; Yanan Yang³; Mark Sartain³; Maya Kasowski⁴; Michael Snyder¹; ¹Department of Genetics, Stanford University, Stanford, CA; ²Agilent Technologies, Wilmington, DE; ³Agilent Technologies, Santa Clara, CA; ⁴School of Medicine, Pathology, Stanford University, Stanford, CA
- WP 565 **Rethinking lipidomic sample normalization: Using the sulfo-phospho-vanillin assay for lipid pre-quantitation in untargeted LC-MS/MS lipidomic applications;** Laura Bailey¹; Kari B Basso²; ¹University of Florida, Gainesville, Florida; ²University of Florida, Gainesville, FL
- WP 566 **Comparison of online and offline HILIC and C30 Reverse Phase Liquid Chromatography coupled to Accurate MS for Quantitative Lipidomic Analysis;** Thu Huong (Nicole) Pham¹; Raymond Thomas²; Lakshman W Galagedara³; ¹Memorial University of Newfoundland, Corner Brook, NL; ²Department of Biology, Faculty of Science, Western University, London, ON; ³School of Science and the Environment, Grenfell Campus, Memorial University of Newfoundland, Corner Brook, NL
- WP 567 **A lipidomics atlas of the diabetic liver in mice;** Meixia Pan¹; Juan Pablo Palavicini¹; Xinlin Han¹; ¹Barshop Institute for Longevity and Aging Studies, University of Texas Health Science Center at San Antonio, San Antonio, Texas
- WP 568 **The effects of systemic lupus erythematosus (SLE) on unsaturated lipids uptakes and their oxidative metabolism in the western population;** Elham Pourmand¹; Kin Sing Lee¹; James Pestka¹; Jenifer Fenton¹; Emily Somers²; Faith Strickland²; Tracy Fuller²; Angel Edwards¹; Suzu Thompson¹; ¹Michigan State university, EAST LANSING; ²University of Michigan-Ann Arbor, Ann Arbor, MI
- WP 569 **Metabolomics Evaluation of the Impact of Violet-Blue Light (405 nm) on Platelet Concentrate;** Jinchun Sun¹; Neetu Dahiya²; Tom Schmitt¹; Caitlin Stewart³; John Anderson³; Scott MacGregor³; Michelle MacLean³; Richard Beger¹; Chintamani D. Atreya²; ¹NCTR / USFDA, Jefferson, AR; ²Office of Blood Research and Review, Center for Biologics Evaluation and Research, United States Food and Drug Administration, Silver Spring, MD; ³The Robertson Trust Laboratory for Electronic Sterilization Technologies, Department of Electronic and Electrical Engineering, University of Strathclyde, Glasgow, United Kingdom
- WP 570 **A high-resolution LC-MS based metabolomics method for spent media analysis in biopharmaceutical cell culture process;** Xiaoli Gao¹; George Gonyea¹; Keegan Orzechowski¹; Alena La¹; Nafees Norris¹; Juan Aon¹; Matthew Maust¹; ¹GSK, Collegeville, Pennsylvania
- WP 571 **Combined GC-TOF-MS and LC-TOF-MS/MS Untargeted Metabolomics Yields Insight into Pathophysiology of Parkinson's Disease;** Lina Dahabiyeh^{1,2}; Jeremiah D Wells¹; Refat Nimer³; Oliver Fiehn¹; ¹University of California, Davis, Davis, CA; ²The University of Jordan, Amman, Jordan; ³Jordan University of Science and Technology, Irbid, Jordan
- WP 572 **Untargeted metabolomic and proteomic analysis of proximal and distal locations in colon and fecal samples by LC-MS/MS;** Oriana Zambito¹; Leanne Ohlund¹; Nejia Lassoued²; Rodolphe Soret^{2,3}; Nicolas Pilon^{2,3}; Lekha Sleno^{1,3}; ¹University of Quebec in Montreal (UQAM), Chemistry department, Montreal, QC; ²University of Quebec in Montreal (UQAM), Biology Department, Montreal, QC; ³CERMO-FC, Centre d'Excellence de Recherche sur les Maladies Orphelines-Fondation Courtois, Montreal, QC
- WP 573 **Combining real time and post-acquisition quality control (QC) for metabolomics workflows;** Aiko Barsch¹; Patrick Groos²; Nikolas Kessler²; Matthias Szesny²; Sven W. Meyer²; Ilmari Krebs²; Heiko Neuwege²; Matthew R Lewis²; ¹Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ²Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- WP 574 **Development of an Offline Two-dimensional LC-MS Method for Chemical Isotope Labeling (CIL)-Based Metabolome Profiling;** Sicheng Quan¹; Shuang Zhao^{1,2}; Liang Li^{1,2}; ¹University of Alberta, Edmonton, AB; ²The Metabolomics Innovation Centre (TMIC) - University of Alberta, Edmonton, AB
- WP 575 **Using Multiple Serum Sample Cohorts with Chemical Isotope Labeling LC-MS to Discover Biomarkers of Rheumatoid Arthritis with Different Seropositivity Status;** Xiaohang Wang¹; Wei Han¹; Walter P. Maksymowych²; Liang Li^{1,3}; ¹The Metabolomics Innovation Centre (TMIC), Edmonton, AB; ²Canadian Research and Education (CaRE) Arthritis, Edmonton, AB; ³Department of Chemistry, University of Alberta, Edmonton, AB
- WP 576 **Optimization of mass spectrometric parameters in data dependent acquisition for untargeted metabolomics;** Hailemariam Abrha Assress^{1,2}; Mario G Ferruzzi^{1,2}; Renny S Lan^{1,2}; ¹University of Arkansas for Medical Sciences, Little Rock, AR; ²Arkansas Children's Nutrition Center, Little Rock, AR
- WP 577 **A biological model of the ageing metabolome reveals potential clinically relevant biomarkers;** Domenica Berardi¹; Emily G Armitage²; Simon Ashton²; Alan Barnes²; Neil Loftus²; Gillian Farrell¹; Abdullah Al Sultan¹; Ashley McCulloch¹; David Watson¹; Matthew Baker³; Zahra Rattray¹; Nicholas JW Rattray¹; ¹Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, Glasgow, United Kingdom; ²Shimadzu Corporation, Manchester, United Kingdom; ³School of Medicine, Faculty of Clinical and Biomedical Sciences University of Central Lancashire, Preston, United Kingdom
- WP 578 **Untargeted spatial metabolomic analysis on Ankylosing Spondylitis preclinical model using MALDI-FTICR-Mass Spectrometry Imaging – Novel analysis approach for biomarker discovery;** Adele-Asia Ponzoni^{1,2}; Silvia Specca³; Amandine Gerstenberg¹; Aureore Tomezyk¹; Mathieu Gaudin¹; Rebecca Deprez-Poulain^{2,4}; David Launay³; Benoit Deprez⁴; Corinne Ramos^{1,2}; ¹ImaBiotech, Loos, France; ²CAPSTONE-ETN MSCA network, Lille, France; ³Institute for Translational Research in Inflammation (INFINITE), U1286, Univ. Lille, Inserm, CHU Lille, Lille, France; ⁴Drugs and Molecules for Living Systems, U1177, Univ. Lille, Inserm, Institut Pasteur de Lille, Lille, France

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- WP 579 **Quantifying spatial and temporal changes of Populus root exometabolites during nutrient-deprived growth conditions;** Manasa R. Appidi^{1,2}; Sameer Mudbhari^{1,2}; Kevin Cope²; Dana L. Carper²; Richard J. Giannone²; Udaya C. Kalluri²; Robert L. Hettich^{1,2}; Paul Abraham^{1,2}; ¹Graduate School of Genome Science and Technology, University of Tennessee, Knoxville, TN, USA, Knoxville, Tennessee; ²Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA, Oak Ridge, Tennessee
- WP 580 **Non-targeted LC-MS analysis of indoor dust in cockroach-infested households;** Daniel Krakko¹; Whitney L. Stutts¹; Madhavi Kakumanu²; Coby Schal²; ¹Molecular Education, Technology and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC; ²Department of Entomology and Plant Pathology, North Carolina State University, Raleigh, NC
- WP 581 **Untargeted Metabolomic Profile of Kaposi's Sarcoma-Associated Herpesvirus (KSHV) Infection by Reversed phase Liquid Chromatography-High-Resolution Mass Spectrometry (LC/HRMS);** Abdulkarim M. Alfaez¹; Bernadett Papp²; Timothy J. Garrett³; ¹University of Florida, Gainesville, Florida; ²University of Florida College of Dentistry, Gainesville, FL; ³University of Florida, Gainesville, FL
- WP 582 **Application of Chemical Isotope Labelling LC-MS Metabolomics to Bovine Pregnancy Investigation;** Daniel Patience¹; Shuang Zhao¹; Marcos Colazo²; Graham Plastow²; Elda Dervishi²; Liang Li^{1,3}; ¹The Metabolomics Innovation Centre (TMIC), Edmonton, AB; ²Department of Agricultural, Food and Nutritional Science, University of Alberta, Edmonton, AB; ³Department of Chemistry, University of Alberta, Edmonton, AB
- WP 583 **Iron Status in Early-Life Modulates Fecal Metabolomics in a Mouse Model;** Anastasiia Kostenko¹; Hui Zhi²; Manuela Raffatellu²; Pieter C. Dorrestein^{3,4}; Allegra T. Aron¹; ¹Department of Chemistry and Biochemistry, University of Denver, Denver, CO; ²Department of Pediatrics, University of California San Diego, La Jolla, CA; ³Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; ⁴Collaborative Mass Spectrometry Innovation Center, University of California San Diego, La Jolla, CA
- WP 584 **Analysis of Anaplerotic Metabolic Incorporation of Dodecanedioic Acid in Cellular Model of Skin Fibroblasts;** Igor Radzikh¹; Yana Sandler¹; ¹Cleveland State University, Cleveland, OH
- WP 585 **Untargeted Urinary Metabolomic Profiling of Patients With Medium-Chain Acyl-Coenzyme A Dehydrogenase Deficiency;** Patrick T. Stumps¹; Pranoot Tanpaiboon¹; Denise Z. Salazar¹; Scott M. Goldman¹; Nigel J. Clarke¹; ¹Quest Diagnostics, San Juan Capistrano, CA
- WP 586 **Using linkage patterns to validate Internal Standard to natural-abundance Isotopic Envelope paired systems;** Chris Beecher¹; Felice De Jong¹; ¹IROA Technologies, Chapel Hill, NC
- WP 587 **Untargeted metabolomics of Bombus impatiens short-term responses to cold exposure via GC-MS;** Hunter Taylor¹; Keaveny Ellen¹; Michael Dillon¹; Franco Basile¹; ¹University of Wyoming, Laramie, WY
- WP 588 **Serum Metabolomics and Lipidomics Studies to Identify Biomarkers for Hepatocellular Carcinoma;** Md Mamunur Rashid¹; Rency S. Varghese¹; Habtom Ressom¹; ¹Georgetown University, Washington, DC
- WP 589 **Sexual Dimorphism of Rewarding System in Mouse Brain Revealed by Parallel Metabolomics and Lipidomics;** Huaxu Yu¹; Tao Huan¹; ¹University of British Columbia, Vancouver, BC
- WP 590 **Tracing the origin of Chinese lotus root varieties using high-resolution mass spectrometry;** Jiao Liu¹; Liqing Zhao²; Jinmei Chen²; Zong Yang²; Bingjie Liu³; Lihai Guo³; ¹Hubei Academy of Agricultural Sciences, Wuhan, China; ²SCIEX, Shanghai, China; ³SCIEX, Beijing, China
- WP 591 **Spatial metabolomics of polymicrobial wound infections and associated adhesive bandages;** Monica Ness¹; Avery Holmes²; Laura-Isobel McCall^{2,3}; Carolyn Ibberson²; ¹University of Oklahoma, Norman, OK; ²University of Oklahoma, Department of Microbiology and Plant Biology, Norman, OK; ³University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK
- WP 592 **Leveraging TENG-MS Untargeted Lipidomics to Study Mesenchymal Stromal Cell Senescence at Low Sample Volumes;** Joseph L. Corstvet¹; Daniel D. Vallejo¹; Molly E. Ogle¹; Johnna S. Temenoff¹; Facundo Fernandez¹; ¹Georgia Institute of Technology, Atlanta, GA
- WP 593 **Segment Scan Mass Spectral Acquisition for Increasing Metabolite Detectability in Chemical Isotope Labeling LC-MS Metabolome Analysis;** Chu-Fan Wang¹; Liang Li¹; ¹Department of Chemistry, University of Alberta, Edmonton, AB
- WP 594 **Developing Workflows to Effectively Probe the Cheese Rind Microbiome Metabolome;** Celine A. Ertekin¹; Laura Sanchez¹; Gordon Luu¹; ¹University of California, Santa Cruz, Santa Cruz, CA
- WP 595 **Study of changes in amyloid protein conformations upon metal binding using top-down protein analysis with TIMS-FTICR-MS;** Francesca O. Bellingeri¹; Meng Li¹; Yuko P. Y. Lam¹; Christopher A. Wootton²; Mark P. Barrow¹; Joanna F. Collingwood¹; Peter B. O'Connor¹; ¹University of Warwick, Coventry, United Kingdom; ²Bruker Dalton's GmbH & Co KG, Bremen, Germany
- WP 596 **CSF proteomic identification of disease-associated protein networks that distinguish between parkinsonian disorders;** Sophia Weiner¹; Mathias Sauer²; Julius Constantinescu³; Radu Constantinescu³; Kaj Blennow^{1,2}; Henrik Zetterberg^{1,2,4,5,6,7}; Johan Gobom^{1,2}; ¹Institute of Neuroscience and Physiology, Department of Psychiatry and Neurochemistry, University of Gothenburg, Mölndal, Sweden; ²Clinical Neurochemistry Lab, Institute of Neuroscience and Physiology, Sahlgrenska University Hospital, Mölndal, Sweden; ³Institute of Neuroscience and Physiology, Department of Neurology, the Sahlgrenska Academy at the University of Gothenburg, Gothenburg, Sweden; ⁴Department of Neurodegenerative Disease, UCL Institute of Neurology, London, United Kingdom; ⁵UK Dementia Research Institute, London, United Kingdom; ⁶Hong Kong Center for Neurodegenerative Diseases, Hong Kong, China; ⁷Wisconsin Alzheimer's Disease Research Center, University of Wisconsin School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI
- WP 597 **Protein and Peptide Signatures Separate Healthy Aging, Mild Cognitive Impairment and Alzheimer's Disease in a Paired CSF and Plasma Study;** Marco Tognetti¹; Yuehan Feng¹; Roland Bruderer¹; Dominique Kamber¹; Jacqueline Darrow²; Alexandra Lewis²; Abhay Moghekar²; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland; ²Johns Hopkins University School of Medicine, Baltimore, MD
- WP 598 **Challenges in hypothesis building through multi-omics analysis of Alzheimer's disease plasma;** Yoshiya Oda¹; Suzumi M. Tokuoka¹; Fumie Hamano¹; Shumgo Adachi²; Tomohiro Andou³; Toru Natsume²; ¹The University of Tokyo, Tokyo, Japan; ²National Institute of Advanced Industrial Science and Technology, Tokyo, Japan; ³Axcellead Drug Discovery Partners Inc., Fujisawa, Japan
- WP 599 **Global and targeted proteomics analysis of mitophagy-associated PINK1, PARKIN, and USP30 substrates upon USP30 inhibition;** Bryan Fonslow¹; Bryan Boyd¹; Nhi Ngo¹; Rachel Herbst¹; Jacquelyn Ha¹; Tina Charlotte Stummann²; Micah Niphakis¹; ¹Lundbeck La Jolla Research Center, Inc., San Diego, CA; ²H. Lundbeck A/S, Valby, Denmark
- WP 600 **Laser capture microdissection (LCM) enriched transcriptome and proteome differences between**

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- substantia nigra and ventral tegmental area human midbrain dopamine neurons; Rahul A Bharadwaj; Lieber Institute for Brain Development, Baltimore, MD**
- WP 601 **Using Native Mass Spectrometry to Deduce the Sizes of Amyloidogenic Protein Oligomers Linked to Neurodegenerative Diseases; Eileen Jacqueline Olivares¹; Carter Lantz¹; Rachel R. Ogorzalek Loo¹; Joseph A. Loo¹; ¹University of California, Los Angeles, Los Angeles, CA**
- WP 602 **Deep phosphoproteomic investigation of reactive primary astrocytes with implications in neuroinflammation through serial metal-affinity-capture (SMAC) single-shot DIA mass spectrometry (DIA-MS); Mahmud Hossain¹; Francesca Rapino¹; Dmitry Ofengeim¹; Nellwyn Hagan¹; Bailin Zhang¹; Dhiman Ghosh¹; ¹Sanofi, Cambridge, MA**
- WP 603 **Detection of epoxides and vicinal diols of docosaehaenoic acid in rat retinas by LC/MS/MS; Genevieve E James¹; Secilia Garza¹; Hikyu Park^{1,2}; Paul Baker³; Mikhail Shchepinov⁴; J. Thomas Brenna^{1,2}; ¹University of Texas at Austin, Austin, TX; ²Dell Medical School, Department of Pediatrics, Austin, TX; ³Sciex, Framingham, MA; ⁴Biojiva, Los Altos, California**
- WP 604 **Understanding Lipid Accumulation in and Around Amyloid Plaques Using Nano-DESI Mass Spectrometry Imaging; Manxi Yang¹; Emerson Hernly¹; Palak Machanda¹; Kaushik Sharma¹; Connor Beveridge¹; Mushfeqa Iqfath¹; Matthew Muhoberac¹; Gaurav Chopra¹; Julia Laskin¹; ¹Purdue University, West Lafayette, IN**
- WP 605 **Characterization of brain O-glycosylation of mice with depressive-like behavior; Youngsuk Seo¹; Boyoung Lee¹; ¹Center for Cognition and Sociality, Institute for Basic Science, Daejeon, South Korea**
- WP 606 **Brain region-specific Lipidomics Profiling of Lipid Droplets in Alzheimer's Disease and Aging; Caitlin E. Randolph¹; Palak Manchanda¹; Connor Beveridge¹; Kanchan Bisht¹; Berwyck Poad²; Stephen J Blanksby²; Gaurav Chopra¹; ¹Purdue University, WEST LAFAYETTE, IN; ²Queensland University of Technology, Brisbane, Australia**
- WP 607 **Qualification of an Immunoaffinity Capture-Liquid Chromatography-Tandem Mass Spectrometry (IAC-LC-MS/MS) Assay to Quantify Huntingtin Protein in Human Peripheral Blood Mononucleocytes (PBMCs); Serge Zemerov¹; Lana Fabia¹; Emma Gromacki¹; Richard C. King¹; Todd Herbst²; Celia Dominguez²; Edith Monteagudo²; Carmen Fernández-Metzler¹; ¹PharmaCadence Analytical Services, LLC, Hatfield, PA; ²CHDI Foundation, Los Angeles, CA**
- WP 608 **A Comparative Proteomic Analysis of Parkinson's Disease, Dementia with Lewy Bodies and Multiple Systems Atrophy; Sinead Greally¹; Mukesh Kumar¹; Christoph N Schlaffner¹; Sabina Berretta²; Hanno Steen³; Judith Steen¹; ¹Boston Children's Hospital, Boston, MA; ²Harvard Brain Tissue Resource Center (HBTRC), McLean Hospital, Belmont, Boston, MA; ³Boston Childrens Hospital, Boston, MA**
- WP 609 **Dissecting Alzheimer's Disease (AD) brains with X-ray Phase-contrast microtomography combined with MALDI-Mass Spectrometry Imaging; Masaya Ikegawa¹; Soichiro Tokuhira¹; Yumiko Toyama¹; Takashi Nirasawa²; Masato Hoshino³; Motohiro Nishikawa⁴; Nobuto Kakuda¹; Yuko Saito⁵; Shigeo Murayama⁵; ¹Doshisha University, Kyotanabe City, Japan; ²Bruker Japan K.K., Yokohama, Japan; ³Japan Synchrotron Radiation Research Institute (JASRI/SPring-8), Harima, Japan; ⁴Kyoto Institute of Nutrition & Pathology, Kyotanabe City, Japan; ⁵Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Itabashi, Japan**
- WP 610 **The Fragile X Glycoproteome: Mass Spectrometric Investigation of Altered Synaptic Plasticity; Ashley Phetsanthad¹; Elliot Patrenets¹; Caroline Roycroft¹; Hannah N. Miles¹; Min Ma¹; Pamela R. Westmark¹; Cara J. Westmark¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI**
- WP 611 **A systematic method to quantify peptides in CSF for the analysis of neurodegenerative diseases; Gennifer Merrihew¹; Jea Park¹; Deanna Plubell¹; Julia E Robbins¹; Brian C Searle²; Eric Huang¹; Christine C. Wu¹; Kathleen Poston³; Thomas J. Montine³; Michael J. MacCoss¹; ¹University of Washington, Seattle, WA; ²Ohio State University, Columbus, OH; ³Stanford University, Stanford, CA**
- WP 612 **Identification of Spontaneous Chemical Modifications in Neurodegenerative Disease Brain Tissue; Brielle L Van Orman¹; Ibrar Siddique²; Gal Bitan²; Blaine Roberts³; Ryan R. Julian¹; ¹University of California, Riverside, Riverside, CA; ²University of California, Los Angeles, Los Angeles, CA; ³Emory University, Atlanta, GA**
- WP 613 **Tissue Specific Interactome of the NPC1 Cholesterol Transporter; Roshan Javanshad¹; Thu T. A. Nguyen¹; Stephanie M Cologna¹; ¹University of Illinois at Chicago, Chicago, IL**
- WP 614 **Spatiotemporal Proteomics of Human iPSC-derived Neuron Model of Frontotemporal Dementia; Wan Nur Atiqah Mazli¹; Jiawei Ni¹; Ashley Frankenfield¹; Ling Hao¹; ¹Department of Chemistry, George Washington University, Washington, DC**
- WP 615 **Spatial proteomic characterization of amyloid plaques in murine Alzheimer's disease brains by laser capture microdissection and mass spectrometry; Mengqi Chu¹; Huan Sun¹; Yun Jiao¹; Junmin Peng¹; ¹Stjude children research hospital, Memphis, TN**
- WP 616 **Comprehensive analysis of protein glycosylation and glycation reveals pathways associated with cognitive decline and protection from cognitive decline; David Morgenstern¹; Hila Levy²; Nili Tickoysky^{3,4}; Lei Yu⁵; Aron S. Buchman⁵; David A. Bennet⁵; Michal Schneider Beer^{3,6}; Yishai Levin²; ¹Weizmann Institute, Rehovot, Israel; ²Weizmann Institute of Science, Rehovot, Israel; ³The Joseph Sagol Neuroscience Center, Sheba Medical Center, Ramat Gan, Israel; ⁴The Goodman faculty of life sciences, Bar Ilan University, Ramat Gan, Israel; ⁵Rush Alzheimer's Disease Center, Rush University, Chicago, IL; ⁶Icahn School of Medicine at Mt Sinai, New York, New York, United States, NY**
- WP 617 **Local and global functional protein networks in Huntington's disease animal models; Todd M. Greco¹; Joshua L Justice¹; Josiah E Hutton¹; Tavis J Reed¹; Jeffrey P Cantle²; Michelle A Kennedy¹; Bokai Song¹; Alma M Perez^{3,4}; Ismael Al-Ramahi^{3,4}; Juan Botas^{3,4}; Jeffrey B Carroll⁵; Ileana M Cristea¹; ¹Princeton University, Princeton, NJ; ²Western Washington University, Department of Psychology, Bellingham, WA; ³Jan and Dan Duncan Neurological Research Institute, Houston, TX; ⁴Baylor College of Medicine, Department of Molecular and Human Genetics, Houston, TX; ⁵University of Washington, Department of Neurology, Seattle, WA**
- WP 618 **Amyotrophic Lateral Sclerosis-associated Mutants of SOD1 Modulate miRNA Biogenesis through Aberrant Interactions with Exportin 5; Xingyuan Chen¹; Xiaomei He¹; Yen-Yu Yang¹; Yinsheng Wang¹; ¹University of California, Riverside, Riverside, CA**
- WP 619 **Deep intact proteoform quantification of microgram-scale proteome by tandem mass tag labeling and online 2D high-pH/low-pH-RPLC top-down analysis; Yanting Guo¹; Trishika Chowdhury¹; Walter P. Galie¹; Kellye A. Cupp-Sutton¹; Dahang Yu¹; Si Wu¹; ¹University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK**
- WP 620 **Analysis of the Δ nox Caulobacter crescentus proteome and c-di-GMP pools using LC-MS; Cameron C Lee-Lopez¹; Md. Shariful Islam¹; Erik T Yukl¹; ¹New Mexico State University, Las Cruces, NM**

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- WP 621 **Long-term quantitative and qualitative reproducibility of capillary zone electrophoresis-tandem mass spectrometry for top-down proteomics of complex proteome samples;** Amirhossein Sadeghi¹; Qiany Wang¹; Wenrong Chen²; Xiaowen Kevin Liu³; Liangliang Sun¹; ¹Michigan State university, EAST LANSING; ²Indiana University Purdue University Indianapolis, Indianapolis, IN; ³Tulane Center for Biomedical Informatics and Genomics, Tulane University, New Orleans, LA
- WP 622 **A multi-layered proteomic atlas to delineate RAS-dependent cellular networks across RAS mutants and isoforms;** Syed Azmal Ali¹; Karim Aljakouch^{1,2}; Jeroen Krijgsveld^{1,2}; ¹German Cancer Research Center, Heidelberg, Germany; ²Heidelberg University, Heidelberg, Germany
- WP 623 **Exploring RNA Binding Interactome in Mouse Macrophages;** Matthew J Marino¹; Deepali Rathore²; Aleksandra Nita-Lazar²; ¹National Institute of Health, Bethesda, MD; ²NIH/NIAID, Bethesda, MD
- WP 624 **Label-Free Quantitation of Protein Mixtures using Data-Independent Acquisition (DIA);** Randy J Arnold¹; Takeshi Shibata²; Ushio Takeda²; Haruka Kumabe³; Takeshi Masuda³; Sumio Ohtsuki³; Patrick Pribil⁴; ¹SCIEX, Bloomington, IN; ²K. K. AB SCIEX, Tokyo, Japan; ³Kumamoto University, Kumamoto, Japan; ⁴SCIEX, Concord, ON
- WP 625 **QCQuan: a new tool for rapid quality assessment of quantitative proteomics experiments;** Simon Appeltans¹; Joris Van Houtven¹; Jef Hooijberghs¹; Dirk Valkenborg¹; ¹Hasselt University - DSI, Hasselt, Belgium
- WP 626 **Brain Organoids in Space: a neurodevelopment proteomic experiment on the effects of microgravity using Cubelab in the International Space Station;** Aline M.A. Martins¹; Livia Luz²; Diego Assis³; Daniel B. McClatchy¹; Jolene K. Diedrich¹; Alysson Muotri²; John Robert Yates III¹; ¹The Scripps Research Institute, La Jolla, CA; ²Sanford Consortium for Regenerative Medicine, UCSD, San Diego, CA; ³Bruker Daltonics, San Jose, CA
- WP 627 **A complementary ion-based strategy enables multiplexed quantification in ETD analysis using DiLeu isobaric tags;** Ting-Jia Gu¹; Peng-Kai Liu²; Danqing Wang³; Zichong Li⁴; Lingjun Li^{1,2,3}; ¹School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ²Biophysics Program, University of Wisconsin-Madison, Madison, WI; ³Department of Chemistry, University of Wisconsin-Madison, Madison, WI; ⁴University of Texas at Austin, Austin, TX
- WP 628 **Targeted quantification of human and mouse Kv7.2 and Kv7.3 in stably transfected HEK293 cells, mouse and rat brains using MRM;** Rainbow WP Kwan¹; Stephanie Lee¹; Gina De Boer¹; Janette Mezeyova¹; Richard Dean¹; Shohei Iwamoto²; Luis Sojo¹; ¹Xenon Pharmaceuticals, Burnaby, BC; ²University of Victoria, Victoria, BC
- WP 629 **Identification of proteins that differentially interact with the phosphorylated and unphosphorylated C-terminal domain of RNA Polymerase 2;** Aarti Bashyal¹; Mukesh K. Venkat Ramani²; Yan Zhang²; Jennifer S. Brodbelt¹; ¹Department of Chemistry, The University of Texas at Austin, Austin, TX; ²Department of Molecular Biosciences, The University of Texas at Austin, Austin, TX
- WP 630 **Proteomics and honey bee health;** Renata Moravcova¹; Kyung-Mee Moon¹; Greg R. Stacey¹; Jason C. Rogalski²; Xiaojing Yuan²; Stephen F. Pernal³; Marta M Guarna³; Shelley Hoover⁴; Ida M. Conflitti⁵; Amro Zayed⁵; Robert Currie⁶; Pierre Giovenazzo⁷; Mateus Pepinelli⁵; Leonard J. Foster¹; ¹Department of Biochemistry and Molecular Biology, UBC, Vancouver, BC; ²Proteomics Core Facility, UBC, Vancouver, BC; ³Agriculture and Agri-Food Canada, Beaverlodge, AB; ⁴Department of Biological Sciences, University of Lethbridge, Lethbridge, AB; ⁵Department of Biology, York University, Toronto, ON; ⁶Department of Entomology, University of Manitoba, Winnipeg, MB;
- ⁷Département biologie, faculté sciences et genie, Université Laval Québec, Quebec, QC
- WP 631 **Tandem Mass Tag (TMT) Quantitation Using Data Directed Analysis and SELECT SERIESTM MRT Mass Spectrometer ;** Christopher J. Hughes¹; Martin E. Palmer¹; James I. Langridge¹; ¹Waters Corporation, Wilmslow, United Kingdom
- WP 632 **Accurate and precise label-free quantification with comprehensive proteome coverage using a novel HRAM platform;** Zilu Ye¹; Anna Pashkova²; Ulises H. Guzmán¹; Florian Harking¹; Tabiwang N. Arrey²; Hamish Stewart²; Ana Martinez Del Val¹; Yue Xuan²; Eugen Damoc²; Jesper V. Olsen¹; ¹Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- WP 633 **Evaluation of a novel high-resolution accurate mass platform for its application on TMT-based multiplexing of single cells;** Pedro Aragon¹; Valdemaras Petrosius¹; Tabiwang N. Arrey²; Nil Üresin³; Benjamin Furtwängler³; Bo Porse³; Hamish Stewart²; Nicolaie Eugen Damoc²; Vlad Zabrouskov²; Erwin M. Schoof¹; ¹Technical University of Denmark, Kgs. Lyngby, Denmark; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ³BRIC - University of Copenhagen, København, Denmark
- WP 634 **Surfaceome characterization in development of CAR-T therapies;** Ruzena Filandrova^{1,2}; Pauline Douglas^{1,2}; Xueyang Guo²; Theodore B. Verhey^{1,2}; Sorana Morissy^{1,2}; David C Schriemer^{1,2}; ¹Department of Biochemistry and Molecular Biology, University of Calgary, Calgary, AB; ²Arnie Charbonneau Cancer Institute, Cumming School of Medicine, University of Calgary, Calgary, AB
- WP 635 **Real-Time Search improves sensitivity of TMTpro complementary ion quantification;** Alex Johnson¹; Jingjing Huang²; William D. Barshop²; Jesse D. Canterbury²; Vlad Zabrouskov²; Graeme McAlister²; Martin Wühr¹; ¹Princeton University, Princeton, NJ; ²Thermo Fisher Scientific, San Jose, California
- WP 636 **Quaternary amine tags for improved complement-quantitation in proteomics samples;** Nick Brodie¹; David C Schriemer¹; ¹University of Calgary, Calgary, AB
- WP 637 **Quantitative Proteomic Profiling in Brain Subregions of Mice Exposed to Open-Field Low-intensity Blast Reveals Position-Dependent Blast Effects;** Marcus Jackson¹; Shanyan Chen¹; Martin Langenderfer²; Chao Li¹; Heather R. Siedhoff¹; Ashley Balderrama¹; Runting Li¹; Catherine E. Johnson²; C. Michael Greenlief¹; Ibolja Cernak³; Ralph G Depalma⁴; Jiankun Cui¹; Zezong Gu⁵; ¹University of Missouri-Columbia, Columbia, MO; ²Missouri University of Science and Technology, Rolla, MO; ³Mercer University, Columbus, GA; ⁴Department of Veterans Affairs, Washington DC, DC; ⁵University of Missouri, Columbia, MO
- WP 638 **Functionalized Nanoparticles Enable Quantitative and Precise Large-Scale Unbiased, Deep Plasma Proteomics;** Ting Huang¹; Jian Wang¹; Alexey Stukalov¹; Margaret Donovan¹; Shadi Ferdosi¹; Lucy Williamson¹; Seth Just¹; Gabriel Castro¹; Eltahir Elgierari¹; Ryan Benz¹; Yingxiang Huang¹; Khatereh Motamedchaboki¹; Omid C. Farokhzad¹; Serafim Batzoglou¹; Simion Kreimer²; Asim Siddiqui¹; Jennifer E. Van Eyk²; Daniel Hornburg¹; ¹Seer, Inc., Redwood City, CA; ²Cedars-Sinai Medical Center, Los Angeles, CA
- WP 639 **Developing Cell Quenching Method to Facilitate Single Cell Mass Spectrometry Metabolomics Studies;** Deepthi Bhusal¹; Shakya Sankalpani Gunasena Wije Munige¹; Zongkai Peng¹; Zhibo Yang¹; ¹University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK
- WP 640 **Single-Cell Proteomic Analysis of Drosophila Oocytes;** Merin M. Rixen¹; Rachel R. Ogorzalek Loo¹; Joseph A. Loo¹; Margot E. Quinlan¹; ¹UCLA, Los Angeles, CA
- WP 641 **Evaluation of sample preparation methods for single cell MALDI-MS;** Stanislav S. Rubakhin^{1,2}; Jonathan V.

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- Sweedler^{1,2}; ¹*Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana and Champaign, IL;* ²*Beckman Institute, University of Illinois at Urbana-Champaign, Urbana and Champaign, IL*
- WP 642 **Data-Dependent Acquisition with Precursor Coisolation Improves Proteome Coverage and Measurement Throughput for Label-Free Single-Cell Proteomics;** Thy Truong¹; Madisyn Johnston¹; Kei Webber¹; Hannah Boekweg¹; Caleb Lindgren¹; Yiran Liang¹; Alissia Nydeggar¹; Xiaofeng Xie¹; Samuel H Payne¹; Ryan Kelly¹; ¹*Brigham Young University, Provo, UT*
- WP 643 **Development of a single-cell proteomic workflow to study the proteomic profiles of PC-12 differentiation;** Arpa Ebrahimi¹; Stanislaw Stanisheuski¹; Liping Yang¹; Luke C. Marney¹; Kavi Aashish Vaidya¹; Claudia Maier¹; ¹*Oregon State University, Corvallis, OR*
- WP 644 **Improving accuracy of protein quantitation in single-cell proteomics;** Connor A Peterson¹; Hannah Boekweg¹; Samuel H Payne¹; ¹*Brigham Young University, Provo, UT*
- WP 645 **Improving throughput of Single Cell Analysis through Hyperplexing and PairQuant Acquisition with inSeqAPI;** Tommy K. Cheung¹; Hanna G Budayeva²; Ying Zhu¹; Christopher M Rose¹; ¹*Genentech, Inc., South San Francisco, CA;* ²*Genentech Inc., South San Francisco, CA*
- WP 646 **Label free single cell proteomics using thermal inkjet dispensing with single cell sensing system;** Stanislaw Stanisheuski¹; Hyo Sang Jang²; Liping Yang¹; Jeffrey Morre¹; Claudia Maier¹; ¹*Oregon State University, Corvallis;* ²*HP Inc., Corvallis, Oregon*
- WP 647 **High throughput single cell proteomics using ultrashort gradients and Wide-Window Acquisition to reach unprecedented proteome coverage and quantitative accuracy;** Manuel Matzinger¹; Rupert L. Mayer¹; Karl Mechtler¹; ¹*Protein Chemistry Group, IMP, Vienna, Austria*
- WP 648 **High-throughput nano LC-MS for sample-limited proteomics;** Alec C Valenta¹; Christopher Pynn²; Dominic Hoch³; Manuel Matzinger⁴; Rupert L. Mayer⁴; Alexander Makarov⁵; Karl Mechtler⁴; Runsheng Zheng²; ¹*Thermo Fisher Scientific, Somers, NJ;* ²*Thermo Fisher Scientific, Germring, Germany;* ³*Thermo Fisher Scientific, Reinach, Switzerland;* ⁴*Institute of Molecular Pathology, Vienna, Austria;* ⁵*Thermo Fisher Scientific, Bremen, Germany*
- WP 649 **A single-cell metabolomics approach for the study of the medicinal plant Catharanthus roseus;** Anh Hai Vu¹; Carlos Eduardo Rodriguez-Lopez²; Delia Ayled Serna Guerrero²; Sarah Ellen O'Connor¹; Lorenzo Caputi¹; ¹*Department of Natural Product Biosynthesis, Max-Planck Institute for Chemical Ecology, Jena, Germany;* ²*Escuela de Ingenieria y Ciencias, Tecnologico de Monterrey, Monterrey, Mexico*
- WP 650 **Spectral library based Single-cell proteomics resolves cellular heterogeneity;** Lakmini Senavirathna¹; Cheng Ma¹; Ru Chen²; Sheng Pan¹; ¹*The University of Texas Health Science Center at Houston, Houston, Texas;* ²*Baylor College of Medicine, Houston, Texas*
- WP 651 **Increasing Proteomic Depth of Single-Cell Analysis by Feature Matching in diaPASEF Data;** Karl K Krull^{1,2}; Syed Azmal Ali¹; Jeroen Krijgsveld^{1,2}; ¹*German Cancer Research Center (DKFZ), Heidelberg, Germany;* ²*Medical Faculty of Heidelberg University, Heidelberg, Germany*
- WP 652 **Enhancing single-cell proteome coverage with a novel high-resolution accurate mass platform;** Valdemaras Petrosius¹; Tabiwang N. Arrey²; Hamish Stewart²; Nicolaie Eugen Damoc²; Vlad Zabrouskov³; Erwin M. Schoof¹; ¹*Technical University of Denmark, Copenhagen, Denmark;* ²*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany;* ³*Thermo Fisher Scientific, San Jose, California*
- WP 653 **Innovative in-capillary sample processing coupled to high-sensitivity CE-MS analysis to decipher the proteome and N-glycome of single mammalian cells;** Yunfan Gao¹; Anne-Lise Marie¹; Alexander R. Ivanov¹; ¹*Northeastern University, Boston, MA*
- WP 654 **Automated Single-Cell Metabolomics to Map Molecular Transducers of MSC Senescence;** Joseph L. Corstvet¹; Samuel M. Ehrlich¹; Daniel D. Vallejo¹; Molly E. Ogle¹; Bo Yang¹; Alexandra E. Dunnum¹; Mohamed W. Badawy¹; Johnna S. Temenoff¹; Craig R. Forest¹; Facundo Fernandez¹; ¹*Georgia Institute of Technology, Atlanta, GA*
- WP 655 **Pipetting-free single cell analysis with the label-free proteoCHIP and the Evotip adapter for high sensitivity proteomics on the timsTOF SCP;** Christoph Krisp¹; Dorte Bekker-Jensen²; David Hartlmayr³; Anjali Seth³; Moritz Heusel²; Magnus Huusfeldt²; Thorsten Ledertheil¹; Jean-Francois Greisch¹; Andreia Almeida⁴; Jarrod Sandow⁴; Guilhem Tourniaire³; Nicolai Bache²; Markus Lubeck¹; Gary Kruppa⁵; ¹*Bruker Daltonics GmbH & Co.KG, Bremen, Germany;* ²*Evosep, Odense, Denmark;* ³*Cellenion SASU, Lyon, France;* ⁴*IonOpticks Pty Ltd, Melbourne, Australia;* ⁵*Bruker S.R.O., Brno, Czech Republic*
- WP 656 **Pushing the boundaries for robust and high-throughput single cell analysis with Whisper Flow technology powered by dia-PASEF;** Dorte B. Bekker-Jensen¹; Christoph Krisp²; David Hartlmayr³; Anjali Seth³; Ole B. Hoerning¹; Moritz Heusel¹; Magnus Huusfeldt¹; Andreia Almeida⁴; Jarrod Sandow⁴; Markus Lubeck²; Gary Kruppa⁵; Nicolai Bache¹; ¹*Evosep Biosystems, Odense, Denmark;* ²*Bruker Daltonics GmbH & Co. KG, Bremen, Germany;* ³*Cellenion SASU, Lyon, France;* ⁴*IonOpticks Pty Ltd, Melbourne, Australia;* ⁵*Bruker S.R.O., Brno, Czech Republic*
- WP 657 **Algorithmic challenges in single-cell proteomics data analysis;** Hannah Boekweg¹; Samuel H Payne¹; ¹*Brigham Young University, Provo, UT*
- WP 658 **Metabolomic coverage of small cell populations;** Julius Agongo¹; James Edwards¹; ¹*Saint Louis University, Saint Louis, MO*
- WP 659 **Top-Down Proteomics of Human Single Cells using Spray-Capillary Based Microsampling and Online CE-MS Analysis;** Walter Galie¹; Zhitao Zhao¹; Trishika Chowdhury¹; Samin Anjum¹; Yanting Guo¹; Kellye A Cupp-Sutton¹; Si Wu¹; ¹*University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK*
- WP 660 **Applying parallel proteomics and transcriptomics from same single-cells to investigate mitotic regulation;** James M Fulcher¹; Lye Meng Markille²; Hugh D Mitchell²; Sarah M Williams²; Kristin M Engbrecht³; Ronald J Moore⁴; William Chrisler⁴; Joshua Cantlon-Bruce⁵; Johannes W Bagnoli⁵; Anjali Seth⁵; Ljiljana Paša-Tolić²; Ying Zhu²; ¹*Pacific Northwest National Lab, Richland, WA;* ²*Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington;* ³*Nuclear, Chemistry, and Biology Division, Pacific Northwest National Laboratory, Richland, Washington;* ⁴*Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA;* ⁵*Cellenion SASU, Lyon, France*
- WP 661 **How many proteins is enough? The race for utility in single-cell proteomics;** Alyssa A Nitz¹; Jose Humberto Giraldez Chavez¹; Samuel H Payne¹; ¹*Brigham Young University, Provo, UT*
- WP 662 **New functionalities of ms.epfl.ch for advanced on-line processing of High-Resolution MS and MS/MS data;** Daniel Trujillo Ortiz¹; Ricardo dos Reis Silvestre²; Natalia Gasilova¹; Rémi Martinet²; Cyril Portmann²; Luc Patiny¹; Vincent Mutel³; Laure Menin¹; ¹*EPFL SB ISIC-GE, Lausanne, Switzerland;* ²*HES-SO, Fribourg, Switzerland;* ³*Inflamalps SA, Monthey, Switzerland*
- WP 663 **All-biomass carbon nanofiber for matrix-free laser desorption/ionization mass spectrometry;** Haoran Zhang¹; Wenxin Wu¹; Lingjun Li¹; ¹*University of Wisconsin-Madison, Madison, WI*
- WP 664 **Method Validation for the Determination of 11-nor-9-carboxy-Δ9-THC and 11-nor-9-carboxy-Δ8-THC in Human Urine by Liquid Chromatography Coupled to Mass Spectrometry (LC/MS/MS);** Amber Awad¹; Ana

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- WP 665 Celia Grenier Ph.d¹; Lawrence J. Andrade¹; ¹*Dominion Diagnostics, North Kingstown, RI*
Removal Of Potential Pitfalls- Improve Ruggedness of Bioanalytical Method by Focusing On Assay Details; Xiaodong Zhu¹; Jingguo Hou¹; Perry Fan¹; Andrew Cunningham¹; ¹*Worldwide Clinical Trials, Austin, TX*
- WP 666 Mass Spectrometry-guided Synthesis of Iodoacetyl Black Hole Quenchers; Pradnya Patil¹; Karine Bagramyan¹; Daniel Röth¹; Markus Kalkum¹; ¹*City of hope, Duarte, CA*
- WP 667 Two-Dimensional Ion Chromatography Tandem Mass Spectrometric (2D IC-MS/MS) Method for The Analysis of Phosphate Metabolites in Soil Matrix; George Gachumi¹; Aimee Schryer¹; Steven Siciliano¹; ¹*University of Saskatchewan, Saskatoon, SK*
- WP 668 Method Development for quantitative determination of creatine phosphate, creatine and ATP in rat brain by LC-MS/MS; Wen Lu¹; Chia-Yi Kuan²; Siming Wang¹; ¹*Georgia State University, Atlanta, GA*; ²*University of Virginia, Charlottesville, VA*
- WP 669 Development of a Biological Reference Material for Accurate Ephedrine Quantification in Urine Using LC-MS/MS; Inseon Kang¹; Yoondam Seo¹; Hyeon-Jeong Lee¹; Junghyun Son¹; Hophil Min¹; ¹*Korea Institute of Science and Technology, Seoul, South Korea*
- WP 670 Identification of Xenobiotic Plant Metabolites Using Isotopic Enhancement Combined with Plant Cell Culture Experiments; Jesse Balcer¹; Yelena Adelfinskaya¹; Chris J Brown¹; Mike Madary¹; Jeffrey R Gilbert¹; Suresh Annangudi¹; ¹*Corteva Agriscience, Indianapolis, IN*
- WP 671 Prioritization Strategies for Non-Target Screening and Applications to Recycled Textile Analysis of Emerging Contaminants; Drew Szabo¹; Varvara Apostolopoulou Kalkavoura¹; Aji Mathew¹; Anneli Krueve¹; ¹*Stockholm University, Stockholm, Sweden*
- WP 672 Assessment of quantification process and measurement uncertainty for LC-IM-TOFMS analysis of contaminants of emerging concern in river water; Teresa Steininger-Mairinger¹; Sven Kochmann^{1,2}; Tim J. Causon¹; Stephan Hann¹; ¹*Department of Chemistry, University of Natural Resources and Life Sciences (BOKU), Vienna, Austria*; ²*ACIB (austrian centre of industrial biotechnology), Vienna, Austria*
- WP 673 Validation of a Robust Quantitative Oral Fluid LC-MS/MS Method Comprised of 54 Analytes; Phillip Hackett¹; Lawrence J. Andrade¹; Ana Celia Grenier Ph.d¹; Amber Awad¹; ¹*Dominion Diagnostics, North Kingstown, RI*
- WP 674 Improved workflow for urinary glycosaminoglycan disaccharide analysis using AMAC derivatization followed by automated solid phase cleanup and LC-MS/MS analysis; Debasish Ghosh¹; Michael L Neugent²; Karsten Liegmann³; Brian Shofran³; Nicole J. De Nisco²; Vladimir Shulaev¹; ¹*University of North Texas, Denton, TX*; ²*UT Dallas, Richardson, TX*; ³*Tecan, Baldwin Park, CA*
- WP 675 Analytical method for separation of isobaric isomers of Delta 8, 9, and 10 THC and their metabolites utilizing fast LC/MS/MS; Andre Szczesniewski; Agilent Technologies, Wood Dale, IL
- WP 676 An Enhanced Avermectin Method for Characterization of Bovine Pharmacokinetics Utilizing Tandem Mass Spectrometry; Greg Jellick¹; Kim Lohmeyer²; Dee Ellis³; Stephan BH Bach¹; ¹*University of Texas at San Antonio, San Antonio, TX*; ²*USDA-ARS, Kerrville, Texas*; ³*Texas A&M, College Station, TX*
- WP 677 Comprehensive analysis of microplastics and their adsorbed environmental matrix constituents using a combination of thermal desorption and pyrolysis with GCxGC-HRTOFMS; David E Alonso¹; Nick Jones¹; Joseph E Binkley¹; ¹*Leco Corporation, St. Joseph, MI*
- WP 678 Bioanalysis of hydroxyl-dendrimer therapeutics using LC-MS/MS with in-source fragmentation; Jason S Watts¹; Emily Taylor¹; Natacha Le Moan²; Jeff Cleland²; Jennifer Zimmer¹; ¹*Alturas Analytics, Inc., Moscow, ID*; ²*Ashvattha Therapeutics, Redwood City, CA*
- WP 679 Deep structural analysis of glycogen in biological samples and in disease states; Yasmine Bouchibti¹; Cathy Chen²; Carlito B. Lebrilla²; ¹*UC Davis Graduate Studies, Davis, CA*; ²*UC Davis, Davis, CA*
- WP 680 Tryptophan metabolite microLC-MS/MS method development and its application to clinical research on metabolism relating to aging and chronic diseases; Carolina N. Perez¹; John J. Thaden¹; Gabriella A.M. Ten Have¹; Nicolaas E.P. Deutz¹; ¹*Texas A&M University - Center for Translational Research in Aging and Longevity, College Station, TX*
- WP 681 Simultaneous quantitation of multiple excipients in biological formulation by using LC-MS/MS; Nilesch Patil¹; Ashutosh Shelar¹; Samruddha Chavan¹; Nitish Ramchandra Suryawanshi¹; Nitin Shukla¹; Purushottam Sutar¹; Dr. Jitendra Kelkar¹; Dr. Pratap Rasam¹; ¹*Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*
- WP 682 Elucidating Gut Microbial Metabolism with Mass Spectrometry Through 13C Labeled Dietary Fiber; Christopher Suarez¹; Cheng-Yu Weng¹; Chad Masarweh¹; David Mills¹; Carlito Lebrilla¹; ¹*University of California, Davis, Davis, CA*
- WP 683 AQMID-MS determines histone methylation with methyl donors from different metabolic sources; Hui Tang¹; Mark Sowers¹; Kangling Zhang¹; ¹*University of Texas Medical Branch at Galveston, Galveston, TX*
- WP 684 Peak Pair Pruner: an addon to MS-DIAL for peak pair validation and ratio quantification of isotopic labeling LC-MS/MS data; Ryan A Smith^{1,2}; Qibin Zhang^{1,2}; ¹*Center for Translational Biomedical Research, University of North Carolina at Greensboro, North Carolina Research Campus, Kannapolis, NC 28081, USA, Kannapolis, NC*; ²*Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, NC*
- WP 685 Measuring Antimicrobial Resistance in Methicillin-Resistant Staphylococcus aureus using Deuterium Labeling on a Bruker Biotyper MALDI-TOF; Josiah J. Rensner¹; Paul Lueth¹; Bryan Bellaire¹; Young Jin Lee¹; ¹*Iowa State University, Ames, IA*
- WP 686 Mass spectrometric characterization of selectively deuterated native bacterial lipids informs design considerations for lipid deuteration and enhances neutron scattering experiments; Matthew J Keller^{1,2}; Qiu Zhang¹; Brian C Sanders¹; Hugh M O'Neill¹; Robert L Hettich^{1,2}; ¹*Oak Ridge National Laboratory, Oak Ridge, TN*; ²*University of Tennessee, Knoxville, Knoxville, TN*
- WP 687 Hydrogen-Deuterium Exchange of Isotopically Labeled Protein Mixtures; Prabavi S Dias¹; Darby Ball¹; Oladimeji S Olaluwoye¹; Javier Flores¹; Sheena D'arcy¹; ¹*University of Texas at Dallas, Richardson, TX*
- WP 688 Discovery of metabolic signature in hepatic fibrosis and pulmonary fibrosis using 13C-MFA; Mijeong Kim¹; Hyun Ju Yoo¹; ¹*Asan medical center, Seoul, South Korea*
- WP 689 A New Set of Isobaric Labeling Reagents for Quantitative 16-Plex Proteomics; Xiaolian Ning¹; Qidan Li²; Jin Zi²; Zhanlong Mei²; Jie Liu²; Yuxing Zhang²; Mao Bi³; Xingang Liu⁴; Chao Lv⁴; Hequan Yao⁵; Jianguo Sun⁵; Feng Rao³; Shuwei Li^{4,5}; Siqi Liu²; ¹*University of Chinese Academy of Sciences, Shenzhen, China*; ²*BGI Shenzhen, Shenzhen, China*; ³*School of Life Sciences, Department of Biology, Southern University of Science and Technology, Shenzhen, China*; ⁴*Nanjing Apollomics Biotech Inc, Nanjing, China*; ⁵*China Pharmaceutical University, Nanjing, China*
- WP 690 Quantitative flux analysis of compartmentalized NADH metabolism; Yahui Wang¹; Ethan Stancliffe¹; Michaela Schwaiger-Haber¹; Leah P. Shriver¹; Gary J. Patti¹; ¹*washington university in St. Louis, saint louis, MO*
- WP 691 Profiling the human urinary proteome using a dimethyl-based multiplex-DIA workflow; Ericka Itang¹; Marvin

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- Thielert¹; Johannes Müller-Reif^{1,2}; Vincent Albrecht¹; Martin Steger³; Matthias Mann¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²OmicEra Diagnostics GmbH, Planegg, Germany; ³NEOsphere Biotechnologies GmbH, Planegg, Germany
- WP 692 **Data-driven approach to resolve precursor enrichment in metabolic labeling**; Henock M. Deberneh¹; Justin Zhu¹; Rovshan G. Sadygov¹; ¹University of Texas medical branch, Galveston, TX
- WP 693 **Quantifying Protein Synthesis Using Orbitrap Gas Chromatography High-resolution Mass Spectrometry**; Xiaorong Fu¹; Stanislaw Deja²; Justin Fletcher¹; Jeffrey Browning¹; Shawn Burgess¹; ¹UT Southwestern Medical Center, Dallas, TX; ²UT Southwestern Medical Center, Dallas, Texas
- WP 694 **Dual tagging for multiplex quantitative metabolomics using LC-HRMS**; Briana Mwinkom Tengan¹; James Edwards¹; Micheal Armbruster¹; ¹Saint Louis University, St. Louis, MO
- WP 695 **Slow TCA cycle flux implies suppressed ATP production in solid tumors**; Caroline R Bartman^{1,2,3}; Daniel R Weilandt^{1,2,3}; Yihui Shen^{1,2}; Won Dong Lee^{1,2}; Yujiao Han^{3,4}; Tara Teslaa^{1,2}; Connor S.R. Jankowski^{1,2}; Laith Samarah^{1,2}; Noel R Park^{2,4}; Victoria Da Silva-Diz⁵; Maya Aleksandrova⁵; Yetis Gultekin^{6,7}; Argit Marishta^{2,4}; Lin Wang^{1,2}; Lifeng Yang^{1,2}; Shawn Davidson²; Martin Wuehr^{1,4}; Matthew G Vander Heiden^{6,7}; Daniel Herranz⁵; Jessie Yanxiang Guo⁵; Yibin Kang^{3,4}; Joshua D Rabinowitz^{1,2,3}; ¹Department of Chemistry, Princeton University, Princeton, NJ; ²Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ; ³Ludwig Institute for Cancer Research, Princeton University, Princeton, NJ; ⁴Department of Molecular Biology, Princeton University, Princeton, NJ; ⁵Cancer Institute of New Jersey, Rutgers University, New Brunswick, NJ; ⁶Koch Institute for Integrative Cancer Research, Massachusetts Institute of Technology, Boston, MA; ⁷Department of Biology, Massachusetts Institute of Technology, Boston, MA
- WP 696 **Immunoprecipitation Based Chemical Cross-Linking Proteomics studies to identify inflammatory protein networks of Toll like Receptor**; Aurchie Rahman¹; A D A Shahinuzzaman¹; Abu Hena Mostafa Kamal²; Saiful Chowdhury¹; ¹University of Texas at Arlington, Arlington, TX; ²Baylor College of Medicine, Houston, TX
- WP 697 **MitoMap – A three-dimensional landscape of mitochondrial architecture**; Kerem Can Akkaya^{1,2,3}; Ying Zhu¹; Cong Wang¹; Dmytro Puchkov²; Martin Lehmann²; Fan Liu^{1,3}; ¹Department of Structural Biology, Leibniz Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; ²Core Facility Cellular Imaging, Leibniz Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; ³Charité – Universitätsmedizin Berlin, Berlin, Germany
- WP 698 **An integrated nascent proteomics approach to systematically investigate how translation initiation factors shape the cancer proteome**; Toman Borteczen¹; Robert Wolfgang Kalis²; Johannes Zuber²; Jeroen Krijgsveld¹; Torsten Müller¹; ¹German Cancer Research Center (DKFZ), Heidelberg, Germany; ²Institute of Molecular Pathology, Vienna, Austria
- WP 699 **Perseus plugin for circadian multi omics data analysis enables accurate prediction of circadian phase from proteomics data**; Carlo De Nart¹; Fatih Aygenli²; Tanja Bange²; Maria Robles²; Jürgen Cox¹; ¹Max Planck Institute of Biochemistry, Planegg, Germany; ²Institute of Medical Psychology and Biomedical Center, Faculty of Medicine, Ludwig-Maximilians-University, München, Germany
- WP 700 **Spatial proteomics and network analysis of murine skeletal muscle reveals the complex structure of the myotendinous junction**; Luisa Schmidt^{1,2}; Philipp Antczak^{1,3}; Andreas Schmidt¹; Abigail Mackey^{4,5}; Michael Kjaer^{4,5}; Marcus Krüger^{1,2}; ¹CECAD research center, Cologne, Germany; ²Institute for genetics, Cologne University, Cologne, Germany; ³Center for Molecular Medicine Cologne, Cologne, Germany; ⁴ISMC, Department of Orthopedic Surgery, Copenhagen University Hospital - Bispebjerg and Frederiksberg, Copenhagen, Denmark; ⁵Department of Clinical Medicine, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark
- WP 701 **The Synaptic Proteome of Autism Spectrum Disorder Across Postnatal Development in Human Primary Visual Cortex**; Shelby Ruiz-Mitzner¹; Kevin Xu¹; Jin-Hong Du²; Bert Klei³; Bernie Devlin³; Matthew L MacDonald^{1,3}; ¹University of Pittsburgh, Pittsburgh, PA; ²Carnegie Mellon University, Pittsburgh, PA; ³University of Pittsburgh Medical Center, Pittsburgh, PA
- WP 702 **MaxQuantAtlas creates large-scale, accurate cellular protein concentration maps from heterogeneous proteomics data**; Daniela Ferretti¹; Yatao Shi²; Pavel Sinitcyn³; Shivani Tiwary³; Chris Browne²; Scott Rusin²; Eric Kuhn²; Susanne Breikopf²; Sarah Martinez²; Dirk Walther²; Juergen Cox¹; Kirti Sharma²; ¹Max Planck Institute of Biochemistry, Martinsried, Germany; ²Kymera Therapeutics, Watertown, MA; ³Max Planck Institute of Biochemistry, Planegg, Germany
- WP 703 **Proteomic Measurements reveal how the bacterium Thermoanaerobacterium thermosaccharolyticum executes the uptake and metabolism of diverse carbohydrates for eventual bioproduct production**; Megan K Elliott^{1,2}; Kristina T Stephens³; Richard J Giannone¹; Evert K Holwerda³; Robert L Hettich^{1,2}; ¹Oak Ridge National Laboratory, Oak Ridge, TN; ²University of Tennessee, Knoxville, TN; ³Dartmouth College, Hanover, NH
- WP 704 **Development and validation of a multi-omics platform to evaluate compounds in Lead Discovery based on progressable and differentiated cellular phenotypes**; Timothy Hamerly¹; Tao Wang¹; Chris Kwiatkowski¹; Karina Edwards¹; Heidi Van Every¹; Evan Rosa-Roseberry¹; Francesca Zappacosta¹; Joseph Kozole¹; Roland Annan¹; ¹GlaxoSmithKline, Collegeville, PA
- WP 705 **USP7 regulates the ncPRC1 Polycomb axis to stimulate genomic H2AK119ub1 deposition uncoupled from H3K27me3**; Jeroen AA Demmers¹; Ayestha Sijm¹; Yaser Atlasi²; Jan A Van Der Knaap¹; Joyce Wolf - Van Der Meer¹; Gillian E Chalkey¹; Karel Bezstarosti¹; Dick HW Dekkers¹; Wouter AS Doff¹; Zeliha Ozgur¹; Wilfred FJ Van Ijcken¹; Peter CP Verrijzer¹; ¹Erasmus Medical Center Rotterdam, Rotterdam, Netherlands; ²Queen's University Belfast, Belfast, United Kingdom
- WP 706 **Proteomic and Transcriptomic analysis of caste transition and aging in the ponerine ant, Harpegnathos saltator**; Maxxum Fioriti¹; Karl Glstad²; Michael Gilbert¹; Matan Sorek²; Tierney Ganon²; Shelley Berger²; ¹Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; ²Department of Cell and Developmental Biology, University of Pennsylvania, Philadelphia, PA
- WP 707 **Multi-omics Evaluation of Progranulin Deficiency in Human iPSCs, iPSC-derived Neurons, and Mouse Brain**; Gwangbin Lee¹; Haorong Li¹; Cha Yang²; Jiawei Ni¹; Wan Nur Atiqah Mazli¹; Fenghua Hu²; Ling Hao¹; ¹Department of Chemistry, George Washington University, Washington, DC; ²Weill Institute for Cell & Molecular Biology, Cornell University, Ithaca, NY
- WP 708 **Integrating Metabolomics and Systems Biology to enhance Limonene yield from engineered bacterial cultures**; Jasmeet Kaur Khanijou¹; Yan Ting Hee²; Chew Wee¹; Kumar Selvarajoo^{2,3,4}; ¹Singapore Institute of Food and Biotechnology Innovation, Singapore, Singapore; ²Bioinformatics Institute (BII), Agency for Science, Technology and Research (A*STAR), Biopolis, Singapore,

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- Singapore; ³Synthetic Biology Translational Research Program & SynCTI, Yong Loo Lin School of Medicine, National University of Singapore (NUS), Kent Ridge, Singapore, Singapore; ⁴School of Biological Sciences, Nanyang Technological University (NTU), Singapore, Singapore
- WP 709 **Multi-layered Proteomics Analysis of Insulin Signaling in a Hepatic Cell Line Mimicking Insulin Sensitivity and Resistance;** Sarah Hyllekvist Jørgensen^{1,2}; Kristina Bennet Emdal²; Anna-Kathrine Pedersen²; Rita Slaaby¹; Peter Kresten Nielsen¹; Jesper Velgaard Olsen²; ¹Novo Nordisk A/S, Måløv, Denmark; ²Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, København, Denmark
- WP 710 **GoDig-enabled Targeted Proteomics Assays Using a Commercialized TMT-labeled Yeast Standard;** Kevin Dong¹; Qing Yu¹; Steven R. Shuken¹; Edward L Huttlin¹; Steven P Gygi¹; Joao A Paulo¹; ¹Harvard Medical School, Boston, MA
- WP 711 **LC-HRMS Based Proteo-metabolomics to Reveal Molecular Remodeling Underlying Methionine-induced Cell Fate Change in Vertebrate (Frog) Embryos;** Jie Li¹; Kaitlyn E. Stepler¹; Leena R. Pade¹; Camille Lombard-Banek¹; Peter Nemes¹; ¹University of Maryland College Park, College Park, MD
- WP 712 **Method Development for Epitope Mapping of Membrane Proteins Embedded in Virus-Like Particles;** Esther Wolf¹; Lauri Peil²; Joan Teyra²; Mart Ustav Jr. ²; Derek Wilson¹; ¹York University, North York, ON; ²Icosagen, Ossu, Estonia
- WP 713 **Elucidation of the distinct RNA-protein interactomes of SARS CoV-2 genomic and subgenomic RNAs;** Isabella T Whitworth¹; Rachel Knoener¹; Maritza Puray-Chavez²; Peter Halfmann¹; M'bark Baddouh¹; Sofia Romero¹; Mark Scalf¹; Yoshihiro Kawaoka¹; Sebla Kutluay²; Lloyd M Smith¹; Nathan M Sherer¹; ¹University of Wisconsin-Madison, Madison, WI; ²Washington University in St. Louis, St Louis, MO
- WP 714 **LC-UV-MS Analysis of Intact Adeno-Associated Virus (AAV) Vector Capsid Proteins;** Amber D Henry¹; Pei Liu¹; Kevin Ray¹; ¹Sigma Aldrich, St. Louis, MO
- WP 715 **Stability Characterization of Multiple Serotypes of Adeno-Associated Virus Using Charge Detection Mass Spectrometry;** Rachel Koerber¹; Susan Abbatiello¹; Andy Jarrell¹; ¹Waters Corporation, Milford, MA
- WP 716 **Characterization of Adeno-associated viral proteins and related proteoforms using top-down approach on a LC-Orbitrap Tribrid MS platform;** Reiko Kiyonami¹; Kristina Srzentic²; Kenneth Thompson³; Chao Yan Liu³; Min Du⁴; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific, CH-, Switzerland; ³Thermo Fisher Scientific, Frederick, Maryland; ⁴Thermo Fisher Scientific, Cambridge, MA
- WP 717 **Reassessment of excess DNA packaging in Zamilon virophage using charge-independent nano-resonator MS;** Szu-Hsueh Lai^{1,2}; Sandra Jeudy³; Adrien Reynaud⁴; Bogdan Vysotsky⁴; Yohann Couté²; Julia Novion-Ducassous²; Jean-Michel Claverie³; Sébastien Hentz⁴; Chantal Abergel³; Christophe Masselon²; ¹Department of Chemistry, National Cheng Kung University, Tainan, Taiwan; ²UA13, Inserm/CEA/UGA IRIG, Biosciences et bio-ingénierie pour la santé, Grenoble, France; ³CNRS - UMR 7256 – IGS, IMM-FR 3479, IM2B, IOM, Marseille, France; ⁴Université Grenoble Alpes, CEA, LETI, Grenoble, France
- WP 718 **Investigating epitranscriptomic communications between selected neuromodulator and HIV-1 lifecycle in the CNS by MS-based techniques;** Limin Deng¹; Jyotsna Kumar¹; Mikaila French¹; Daniele Fabris¹; ¹UConn Chemisrty Dept., Storrs, CT
- WP 719 **Adeno-Associated Virus Capsid Proteins Peptide Mapping by Analytical & Micro Flow Reversed Phase Chromatography Coupled to High Resolution Mass Spectrometry;** Sergio Guazzotti¹; Roxana Eggleston-Rangel²; Mastroreh Chamanian²; Lorne Nelson²; ¹Phenomenex, Alcobendas, Madrid, Spain; ²Phenomenex, Torrance, CA
- WP 720 **Peptide mapping and post-translational modifications of AAV5 produced in HEK293;** Geoffrey Rule¹; Agnieszka Lass-Napiorkowska²; Pei Liu²; Kevin Ray²; Cory Muraco³; ¹Millipore Sigma, Bellefonte, PA; ²MilliporeSigma, St. Louis, MO; ³MilliporeSigma, Bellefonte, PA
- WP 721 **Detailed Characterization of Adeno-Associated Virus Capsid Proteins by Combining Peptide Mapping and Protein Fingerprinting by Intact Mass;** Kevin Ray¹; Pei Liu¹; ¹MilliporeSigma, St. Louis, MO
- WP 722 **Arboviral-induced alterations of the mosquito lipidome;** Paul S. Soma¹; Oshani Ratnayake¹; Irma Sanchez-Vargas¹; Nunya Chotiwan^{1,2}; Barbara Graham¹; Samantha Pinto¹; Amber Hopf-Jannasch³; Rushika Perera¹; ¹Center for Metabolism of Infectious Diseases, Center for Vector-borne Infectious Diseases, Colorado State University, Fort Collins, CO; ²Chakri Naruebodindra Medical Institute, Faculty of Medicine Ramathibodi Hospital, Thailand; ³Bindley Bioscience Center, Purdue University, West Lafayette, Indiana
- WP 723 **Assessing the fate of Virus-Like-Particles (VLPs) during nebulization before mass analysis;** Vaitson Çumaku^{1,2}; Mehrzad Roudini³; Louis Dartiguelongue²; Bastien Pellegrin⁴; Sébastien Artous²; Andreas Winkler³; Christophe Masselon²; ¹University of Grenoble Alpes (UGA), Grenoble, France; ²CEA, IRIG, Grenoble, France; ³Leibniz Institute for Solid State and Materials Research, IFW Dresden, Dresden, Germany; ⁴CEA, LITEN, Grenoble, France
- WP 724 **Not too heavy, not too light, it's just right! - Using viral molecular mass to discriminate human respiratory viruses;** Vaitson Çumaku^{1,2}; Thomas Fortin²; Sébastien Hentz³; Christophe Masselon²; ¹University of Grenoble Alpes (UGA), Grenoble, France; ²CEA, IRIG, Grenoble, France; ³CEA, LITEN, Grenoble, France
- WP 725 **Optimized Liquid Chromatography-Mass Spectrometry Methods for Intact Protein Analysis and Peptide Mapping of Adeno-Associated Virus Capsid Proteins;** Isin Tuna Sakallioğlu¹; Anjali Alving¹; ¹Bruker Scientific, LLC, Billerica, MA
- WP 726 **Development of an LC-MS/MS Based Multi-Attribute Characterization Assay for a Live Virus Vaccine;** David Foreman¹; Alyssa Q Stiving¹; Xuanwen Li¹; Hillary A. Schuessler¹; ¹Merck, West Point, PA
- WP 727 **Mass Spectrometry-based Determination of Tailed Phage Virion Protein Copy Number;** Gialinh Vu¹; Sophia Unwin¹; Sammy Pardo²; Dana Molleur²; Susan Ludwigsen³; Susan T. Weintraub²; Julie A. Thomas¹; ¹Rochester Institute of Technology, Rochester, NY; ²Univ. of Texas HSC, San Antonio, TX; ³Proteome Software, Portland, OR
- WP 728 **HIV-1 Virion Proteoform Analysis Reveals Conserved and Novel Post-Translation Modifications Modulating Viral Function;** Claire E Boos¹; James W Bruce¹; Mark Scalf¹; Rachel M Miller¹; Nathan M Sherer¹; Lloyd M Smith¹; ¹University of Wisconsin-Madison, Madison, WI
- WP 729 **Individual Ion and Charge Detection on the Orbitrap Analyzer for Robust Analysis of Large Native Complexes;** Jared O. Kafader¹; John P. McGee¹; Pei Su¹; Michael A. R. Hollas¹; Ryan T. Fellers¹; Kenneth R Durbin¹; Philip D. Compton²; Neil L. Kelleher¹; ¹Northwestern University, Evanston, IL; ²Integrated Protein Technologies Inc., Carlsbad, CA
- WP 730 **In-depth Characterization of Adeno-Associated Viruses using Microchip Capillary Electrophoresis Coupled with Mass Spectrometry;** Josh Smith¹; Sara Carillo¹; Adi M Kulkarni²; Erin Redman²; Kate Yu²; Jonathan Bones^{1,3}; ¹National Institute of Bioprocessing Research and Training, Dublin, Ireland; ²908 Devices, Inc., Boston, MA; ³School of Chemical and Bioprocess Engineering, University College Dublin, Dublin, Ireland

WEDNESDAY POSTERS

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

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Antidoping, Cannabis, and Opioid Detection	019-025
Data-Independent Acquisition II	026-046
Education: Teaching MS and Teaching with MS	047-052
Elemental Analysis.....	053-054
Energy: Petroleum, Biofuels, and Algae	055-064
Environmental: General III.....	065-089
Environmental: Pharmaceuticals and Pesticides	090-101
Exposomics.....	102-121
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Small Molecules: Qualitative and Quantitative Analysis II.....	714-735

- ThP 001 **Exploring the Application of Rapid Evaporative Ionisation Mass Spectrometry (REIMS) to Bovine Health Monitoring and Milk Quality Analysis;** Rachel Patricia Murdock¹; Sharon Huws¹; Simon Cameron¹; ¹Queen's University Belfast, Belfast, United Kingdom
- ThP 002 **Rapid, High-Throughput Measurement of Catecholamine Neurotransmitters and Their Metabolites in Urine by Paper Spray Mass Spectrometry (PS-MS);** Taelor M. Zarkovic^{1,2}; Jan Palaty³; Jason L. Robinson⁴; Christopher G. Gill^{1,2,5,6,7}; ¹Appl. Env. Res. Labs. (AERL), Nanaimo, BC; ²University of Victoria, Victoria, BC; ³Fraser Health, New Westminster, BC; ⁴Health PEI, Charlottetown, PEI; ⁵Vancouver Island University, Nanaimo, BC; ⁶Simon Fraser University, Burnaby, BC; ⁷University of Washington, Seattle, WA
- ThP 003 **Can the extracted chemical information from FFPE samples using LA-REIMS imaging support pathological diagnosis?;** Gabriel Stefan Horkovics-Kovats^{1,2}; Richard Schäffer²; Csaba Hajdu²; Attila Egri²; Fanni Csiza³; Bálint András Deák³; Benedek Gyöngyösi³; Gitta Schlosser¹; Julia Balog²; ¹Eötvös Loránd University, Budapest, Hungary; ²Waters Research Center, Budapest, Hungary; ³Department of Pathology, Forensic and Insurance Medicine Semmelweis University, Budapest, Hungary
- ThP 004 **Field Forward Collection and Analysis: Utilizing Pressure-Sensitive Adhesive Paper Combined with Portable Mass Spectrometry for Detection of Threats;** Dan Carmany¹; Nicholas Manicke²; Elizabeth Dhummakupt³; ¹Excet, Gunpowder, MD; ²IUPUI, Indianapolis, IN; ³U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD
- ThP 005 **Identification of Ignitable Liquids by Gas Chromatography-Mass Spectrometry and Direct Analysis in Real-Time-Mass Spectrometry via Their Marker Compounds;** Shruthi Perna¹; Briza Marie Dedicataria²; Ngee Sing Chong²; Mengliang Zhang²; ¹Middle Tennessee State University, Murfreesboro, TN; ²Middle Tennessee State University, Murfreesboro, TN
- ThP 006 **Ambient Ionization-Based Screening Protocols for High Priority N-Nitrosamines in Pharmaceutical, Forensic, and Environmental Samples;** Ebenezer H. Bondzie¹; Trevor J. McDaniel¹; Patrick W. Fedick²; Christopher C. Mulligan³; ¹Illinois state university, Normal, IL; ²Naval Air Warfare Center, Weapons Division, China Lake, CA; ³Illinois State University, Normal, IL
- ThP 007 **Rapid, parallel analysis of derivatized volatile phenols in grapes and wines by sorbent sheets (SPMESH) coupled to DART-MS;** Terry L Bates^{1,2}; Gavin L. Sacks¹; ¹Cornell University, Ithaca, NY; ²Bruker Daltonics, Billerica, MA
- ThP 008 **Biopolymer-based sorptive phases into hypodermic needles: sample preparation and direct ambient mass spectrometry analysis in a single device;** Jaime Millán-Santiago¹; Rafael Lucena¹; Soledad Cárdenas¹; ¹University of Córdoba, Córdoba, Spain
- ThP 009 **Accelerated Aza-Michael Addition and SuFEx Reaction in Microdroplets;** Jyotirmoy Ghosh¹; Joshua Mendoza²; R. Graham Cooks²; ¹Purdue University, West Lafayette, IN; ²Purdue University, WEST LAFAYETTE, IN
- ThP 010 **Differentiation of Poly(vinylidene fluoride) polymers based on their end groups by DART-FT-ICR MS and modified Kendrick mass defect diagram;** Pierre Pacholski^{1,2}; Sébastien Schramm²; Frédéric Progent¹; Frédéric Aubriet²; ¹CEA, DAM, DIF, F-91297 Arpajon, France; ²Laboratoire de Chimie et Physique-Approche Multi-échelles des Milieux Complexes (LCP-A2MC), Université de Lorraine, METZ, France
- ThP 011 **Rapid Detection of Amino Acid-based Metabolic Disorders by On-Sample Schiff Base Derivatization and Paper Spray Mass Spectrometry;** Marcos Bouza Areces¹; Daniel Foest²; Sebastian Brandt²; Juan F. García-Reyes¹; Joachim Franzke²; ¹University of Jaén, Jaén, Spain;

THURSDAY POSTERS

- ²Leibniz Institute for Analytical Sciences - ISAS, Dortmund, Germany
- ThP 012 **Comparison of LC-MS and Two Ambient Ionization Techniques for the Quantitative Analysis of Phenylbutazone and Oxphenbutazone in Equine Serum;** David Borts¹; Laura Burns¹; Dwayne Schrunk¹; Tom Kane²; Ryan Micklitsch²; Shane Stevens²; ¹Iowa State University Veterinary Diagnostic Laboratory, Ames, IA; ²Restek Corporation, Bellefonte, PA
- ThP 013 **Towards mass spectrometry guided skin cancer surgery;** Lauritz Falkow Brorsen^{1, 2, 3}; Fernanda Endringer Pinto²; Martin Glud¹; Stine Regin Wiegell¹; James McKenzie³; Uwe Paasch⁴; Merete Hædersdal¹; Zoltan Takats³; Christian Janfelt²; Catharina Margrethe Lerche¹; ¹Bispebjerg Hospital, Copenhagen, Denmark; ²University of Copenhagen, Copenhagen, Denmark; ³Imperial College, London, London, United Kingdom; ⁴University of Leipzig, Leipzig, Germany
- ThP 014 **Rapid analysis of C6 aldehydes in foodstuffs by sorbent sheet extraction and direct analysis in real time-mass spectrometry (SPMESH-DART-MS);** Andre P. Kalenak¹; Terry L Bates¹; Gavin L. Sacks¹; ¹Cornell University Dept. of Food Science, Ithaca, NY
- ThP 015 **Quantitation of Lignin/Cellulose/Hemicellulose and Lignin Monomeric Unit Ratios in Lignocellulosic Biomass via Laser-Assisted Micro-Pyrolysis Flowing Atmospheric-Pressure Afterglow Mass Spectrometry;** Dong Zhang¹; Michael Loomer¹; Ejoke Akatugba¹; Gerardo Gamez¹; ¹Texas Tech University, Lubbock, TX
- ThP 016 **Direct analysis and classification of different olive oils by paper spray mass spectrometry;** Ines R Talarico¹; Lucia Bartella¹; Priscilla Rocio Bautista²; Antonio Molina Díaz³; Leonardo Di Donna¹; Juan F Garcia-Reyes³; ¹University of Calabria, Rende, Italy; ²Universidad de Jaén, Jaén, Spain; ³UNIVERSITY OF JAEN, Jaen, Spain
- ThP 017 **A Tool Allowing Rapid Acquisition and Extraction for Processing of DESI Screening Application Data;** Mark Towers¹; Lisa Reid¹; Richard Chapman²; Joanne B Ballantyne¹; Royston Goodacre³; Ian D Wilson³; Paul Richardson³; Richard Daw⁴; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters Corporation, Milford, Milford, MA; ³University of Liverpool, Liverpool, United Kingdom; ⁴Waters Corporation, milford, MA
- ThP 018 **4 to 6 Orders of Magnitude More Matter Into The Ion Inlet Tube For IBF "ESI" MS With A Surprise;** Drew Sauter; Nanoliter, LLC, Henderson, NV
- ThP 019 **Simultaneous Analysis of Methadone, Naltrexone, Naloxone and Nalmefene in Dog Plasma using LC-MS/MS;** Rachel M. Proctor¹; Youwen You¹; Jaclyn R. Missanelli¹; Cynthia Otto²; Mary A. Robinson¹; ¹University of Pennsylvania, West Chester, PA; ²University of Pennsylvania, Philadelphia, PA
- ThP 020 **Automating analyses of confiscated samples for identification of illicit drugs;** Fuyu Guan¹; Savannah Fay²; Matthew A. Adreance¹; Leif McGoldrick¹; Rachel M. Proctor¹; Jaclyn R. Missanelli¹; Youwen You¹; Mary A. Robinson¹; ¹University of Pennsylvania, West Chester, PA; ²Katherine A. Kelley State Public Health Laboratory, Rocky Hill, CT
- ThP 021 **Simultaneous Quantification and Confirmation of Oxycodone and its Metabolites in Equine Urine by UHPLC-MS/MS;** Jaclyn R. Missanelli¹; Youwen You¹; Rachel M. Proctor¹; Joanne Haughan¹; Mary A. Robinson¹; ¹University of Pennsylvania, West Chester, PA
- ThP 022 **A novel high-throughput GC-MS/MS method for detecting NSAIDs, Steroids, and Cannabinoids in Equine Plasma;** Leif K McGoldrick^{1, 2}; Youwen You^{1, 2}; Fuyu Guan^{1, 2}; Mary A. Robinson^{1, 2}; ¹Department of Clinical Studies, School of Veterinary Medicine, University of Pennsylvania, New Bolton Center Campus, Kennett Square, PA; ²Pennsylvania Equine Toxicology and Research Laboratory, West Chester, PA
- ThP 023 **HR-MS/MS EAD and CID fragmentation leads to selective, sensitive and reliable quantitation of anabolic steroids in urine;** Adrian Soborń^{1, 2}; Rafał Szewczyk^{1, 2}; Anna Lenartowicz¹; Julia Mironenka¹; Katarzyna Krupczyńska-Stopa^{1, 2}; Maciej Stopa^{1, 2}; Andrzej Kwaśnica³; ¹LabExperts sp. z o. o., Gdańsk, Poland; ²Bioanalytic sp. z o. o., Gdańsk, Poland; ³Lab4Tox sp. z o. o., Wrocław, Poland
- ThP 024 **Multiplex analysis of muscle developing five monoclonal antibodies in human plasma with LC-HRMS;** Hyeon-Jeong Lee^{1, 2}; Yoondam Seo^{1, 3}; Inseon Kang¹; Junghyun Son¹; Eugene C. Yi²; Hophil Min¹; ¹Korea institute of science and technology, Seoul, South Korea; ²Seoul National University, Seoul, South Korea; ³Korea university, Seoul, South Korea
- ThP 025 **Using Water Adduction to Differentiate Cannabinoid Isomers in a Quadrupole Ion Trap Mass Spectrometer;** Dinuri S. Fernando¹; Cameron D. Worthington¹; Gary L. Glish¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, North Carolina
- ThP 026 **Over 150 000 Peptide Precursors Identified in a Single Injection diaPASEF Workflow;** Mahmoudreza Ghaznavi^{1, 2}; Joshua Charkow^{1, 2}; Brendon Seale³; Brett Larson³; Anne-Claude Gingras^{1, 3}; Hannes L Röst^{1, 2}; ¹Department of Molecular Genetics, University of Toronto, Toronto, ON; ²Donnelly Centre for Cellular and Biomolecular Research, University of Toronto Toronto, ON, Canada, Toronto, ON; ³Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Sinai Health, Toronto, ON
- ThP 027 **Quantifying 1000 protein groups per minute of gradient using data-independent acquisition (DIA) on a hybrid quadrupole time-of-flight system;** Nick Morrice¹; Ihor Batruch²; Patrick Pribil²; ¹SCIEX, Macclesfield, United Kingdom; ²SCIEX, Concord, ON
- ThP 028 **Integrating DIA-NN software analysis of data-independent acquisition data into a cloud processing pipeline;** Melanie Juba¹; Nick Morrice²; Alexandra Antonoplis³; Christie Hunter³; Patrick Pribil⁴; ¹SCIEX, Redwood City, CA; ²SCIEX, Alderley Park, United Kingdom; ³SCIEX, Redwood city, CA; ⁴SCIEX, Concord, ON
- ThP 029 **Assessment of an optimized DIA-PASEF method for the detection of low-abundant differential proteins in spike-in experiments;** Jeewan Babu Rijal¹; Christine Schaeffer¹; Christine Carapito¹; ¹Laboratoire de Spectrométrie de Masse BioOrganique, Institut Pluridisciplinaire Hubert Curien (UMR 7178), Strasbourg, France
- ThP 030 **MaxLFQ algorithm enables accurate hybrid precursor-fragment-based quantification of plexDIA data in MaxQuant;** Dmitry Alexeev¹; Juergen Cox¹; ¹Max Planck Institute of Biochemistry, Martinsried, Germany
- ThP 031 **Proteomic turnover and thermal stability profiling of chromosome 3 aneuploidy in lung cancer;** Yi Di^{1, 2}; Wenxue Li^{1, 2}; Joan Josep Castellano Pérez³; Qian Ba¹; Alison M. Taylor³; Yansheng Liu^{1, 2}; ¹Yale University, New Haven, CT; ²Yale Cancer Biology Institute, West Haven, CT; ³Columbia University, New York, NY
- ThP 032 **DIA Phosphoproteomics: Comparative Evaluation of Dynamic Range and Quantitative Accuracy across Multiple MS Platforms;** Tanmayi D Vashist¹; Alvaro Sebastian Vaca^{1, 2}; Claudia Ctordecka¹; Khoi Pham Munchic¹; Hasmik Keshishian¹; D. R. Mani¹; Shankha Satpathy¹; Steven A Carr¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²Bruker Daltonics, Billerica, MA
- ThP 033 **Improved library free dia-PASEF based quantitative proteomics using Spectronaut;** Tejas Gandhi¹; Oliver M Bernhardt¹; Véronique Laforte¹; Damiano Robbiani¹; Anna Susmelj¹; Lukas Reiter¹; ¹Biognosys AG, Schlieren, Switzerland
- ThP 034 **Accelerated mass spectrometry imaging via MS/MS spectrum deconvolution of inter-pixel compositional variations of metabolites;** Dan Li¹; Zheng Ouyang¹; Xiaoxiao Ma¹; ¹State Key Laboratory of Precision

THURSDAY POSTERS

- ThP 035 *Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University,, Beijing, China*
From data-independent acquisition (DIA) to targeted MS/MS: Automatic reinjection for additional confirmation in suspect screening; Christian Klein¹; James S Pyke¹; Emma E Rennie¹; Cate Simmermaker¹; Karen E Yannell¹; Madhusudan Sharma¹; Li Sun¹; Kai Chen¹; ¹*Agilent Technologies, Santa Clara, CA*
- ThP 036 **Comparison of library-free analysis of mice liver proteomics with data-independent acquisition generated by TripleTOF 5600 and ZenoTOF7600;** Chang Liu¹; Tess Puopolo¹; Huifang Li¹; Ang Cai¹; Hang Ma¹; Navindra P Seeram¹; ¹*University of Rhode Island, Kingston, RI*
- ThP 037 **DirectDIA+ improves library free quantification for plasma proteomics;** Damiano Robbiani¹; Tejas Gandhi¹; Lukas Reiter²; Oliver M Bernhardt²; Roland Bruderer¹; ¹*Biognosys AG, Schlieren, Switzerland*; ²*Biognosys AG, Schlieren, Switzerland*
- ThP 038 **Generating fit-for-purpose targeted assays from a catalog of pre-screened peptides using data-independent acquisition (DIA) based figures of merit;** Ariana E Shannon^{1,2,3}; Yi Wang¹; Gang Xin^{1,4}; Amanda B. Hummon^{1,3}; Brian C Searle²; ¹*Pelotonia Institute for Immuno-Oncology, Comprehensive Cancer Center The Ohio State University, Columbus, Ohio*; ²*Department of Biomedical Informatics, The Ohio State University Medical Center, Columbus, Ohio*; ³*Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio*; ⁴*Department of Microbial Infection and Immunity, The Ohio State University Medical Center, Columbus, Ohio*
- ThP 039 **Efficient generation of highly multiplexed serum biomarker panels using gas phase fractionation and DIA libraries;** Abigail Burrows Franco¹; Cecily R Wood¹; Alison Porter¹; Scott M Peterman²; Scott D Stanley¹; ¹*University of Kentucky, Lexington, KY*; ²*Thermo Fisher Scientific, San Jose, CA*
- ThP 040 **Streamlining biomarker discovery with DIA-MS in large prostate cancer fluid-based clinical cohort;** Annie Ha^{1,2}; Amanda Khoo^{1,2}; Zhuyu Qiu³; Vladimir Ignatchenko²; Julius O Nyalwidhe^{4,5}; O. John Semmes⁴; Danny Vesprini^{6,7}; Stanley K. Liu^{1,7,8}; Paul C Boutros^{1,3,9,10,11,12,13}; Thomas Kislinger^{1,2}; ¹*Department of Medical Biophysics, University of Toronto, Toronto, ON*; ²*Princess Margaret Cancer Centre, University Health Network, Toronto, ON*; ³*Jonsson Comprehensive Cancer Center, University of California, Los Angeles, Los Angeles, CA*; ⁴*Department of Microbiology and Molecular Cell Biology, Eastern Virginia Medical School, Norfolk, VA*; ⁵*Leroy T. Canoles, Jr. Cancer Research Center, Eastern Virginia Medical School, Norfolk, VA*; ⁶*Department of Radiation Oncology, Odette Cancer Centre, Sunnybrook, Toronto, Ontario*; ⁷*Department of Radiation Oncology, University of Toronto, Toronto, Ontario*; ⁸*Odette cancer research Program, Sunnybrook research Institute, Toronto, Ontario*; ⁹*Vector Institute for Artificial Intelligence, Toronto, Ontario*; ¹⁰*Department of Human Genetics, University of California, Los Angeles, CA*; ¹¹*Department of Urology, University of California, Los Angeles, CA*; ¹²*Department of Pharmacology and Toxicology, University of Toronto, Toronto, Ontario*; ¹³*Institute for Precision Health, David Geffen School of Medicine, University of California, Los Angeles, CA*
- ThP 041 **Analyzing data-independent acquisition (DIA) data one experimental spectrum at a time;** Daniel P. Zolg¹; Tobias Schmid¹; Siegfried Gessulat¹; Florian Seefried¹; Michael Graber¹; Samia Ben Fredj¹; Patroklos Samaras¹; Markus Schneider¹; Layla Eljagh¹; Vishal Sukumar¹; Pedro Navarro²; Kai Fritze²; Yovany Cordero Hernandez²; Frank Berg²; Carmen Paschke²; David Horn³; Bernard Delanghe²; Christoph Henrich²; Mathias Wilhelm⁴; Martin Heinrich Frejno¹; ¹*MSAID GmbH, Garching b.München, Germany*; ²*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*; ³*Thermo Fisher Scientific, San Jose, CA*; ⁴*Computational Mass Spectrometry, Technical University of Munich, Freising, Germany*
- ThP 042 **Exploring the benefits of differential mobility separation (DMS) and SWATH data-independent acquisition (DIA) for complex proteomic sample analysis;** Yves Le Blanc¹; Eva Duchoslav¹; Lyle Burton¹; Stephen Tate²; Bradley Schneider²; ¹*SCIEX, Concord, ON, ON*; ²*SCIEX, Concord, ON*
- ThP 043 **Investigation of the human lysosomal proteome by targeted proteomics;** Stephanie Kaspar-Schoenefeld¹; Dhriti Arora²; Andreas Schmidt¹; Dominic Winter²; ¹*Bruker Daltonik GmbH & Co. KG, Bremen, Germany*; ²*Institute for Biochemistry and Molecular Biology, Medical Faculty, Rheinische Friedrich-Wilhelms-University of Bonn, Bonn, Germany*
- ThP 044 **Proteomic Strategies Uncover A Novel Aging Phenotype in the Post-Menopausal Ovary;** Christina D King¹; Shweta S Dipali²; Francesca E Duncan^{1,2}; Birgit Schilling¹; ¹*Buck Institute for Research on Aging, Novato, CA*; ²*Northwestern University, Evanston, IL*
- ThP 045 **Benchmarking DIA data analysis workflows;** An Staes^{1,2,3}; Teresa Maia^{1,2,3}; Robbin Bouwmeester^{1,3}; Ralf Gabriels^{1,3}; Lennart Martens^{1,3}; Katie Boucher^{1,2,3}; Simon Devos^{1,2,3}; Kris Gevaert^{1,3}; Francis Impens^{1,2,3}; ¹*VIB-UGent Center for Medical Biotechnology, Gent, Belgium*; ²*VIB Proteomics Core, Gent, Belgium*; ³*UGent Department of Biomolecular Medicine, Gent, Belgium*
- ThP 046 **Label-free quantification of over 5000 protein groups from single-cell sample amounts with median CV approaching 10% using tims-TOF SCP DIA;** Peter M Pichler¹; Manuel Matzinger¹; Goran Mitulovic²; Karl Mechtler¹; ¹*Research Institute of Molecular Pathology, Vienna, Austria*; ²*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*
- ThP 047 **Design of Mass Spectrometry Experiments for Undergraduate Courses;** Jiexun Bu¹; Junhan Wu²; Nan Zhang¹; Yuyu Li¹; Wenpeng Zhang²; Zheng Ouyang²; ¹*PURSPEC Technology (Beijing) Ltd., Beijing, China*; ²*Department of Precision Instrument, Tsinghua University, Beijing, China*
- ThP 048 **Data-centric tutorials for learning mass spectrometry and proteomics;** Ansima R Mongane¹; Luke A Squires¹; Alyssa A Nitz¹; Samuel H Payne¹; ¹*Brigham Young University, Provo, UT*
- ThP 049 **Development of a self-service LC-QTOF-based metabolomics training workflow in an open access core facility** Paul Mathews, Claudia M. Boot; Paul G Mathews¹; Claudia M Boot¹; ¹*Colorado State University, Fort Collins, CO*
- ThP 050 **Benchtop MALDI MSI: Mass Spectrometry Imaging on a Budget;** Kendra G. Selby¹; Emily M Hubecky¹; Gabriel A. Brendendorff¹; Ashley R Chirchirillo¹; Summy Shrestha¹; Lynne Ling²; Donald Caspary²; Kevin R Tucker¹; ¹*Southern Illinois University Edwardsville, Edwardsville, IL*; ²*Southern Illinois University School of Medicine, Springfield, IL*
- ThP 051 **Social Media for Mass Spectrometry;** Kermit K. Murray; ¹*Louisiana State University, Baton Rouge, LA*
- ThP 052 **Unlocking the Power of Mass Spectrometry in Biomanufacturing: A Microlearning Approach;** M. Cyndell Gracieux-Singleton¹; Jason Whitley¹; Brian Herring¹; Marie Vestergaard²; Scott Latus¹; ¹*Biomanufacturing Training and Education Center (BTEC), NCSU, Raleigh, NC*; ²*Technical University of Denmark, Kgs. Lyngby, Denmark*
- ThP 053 **Multi-Elemental Analysis of Chemically Defined Cell Culture Media by ICP-MS;** Yulan Bian¹; Aimei Zou¹; Patrick Simmons²; ¹*Agilent Technologies, Singapore, Singapore*; ²*Agilent Technologies, Santa Clara, CA*
- ThP 054 **Mpx/hr LA-ICP-TOFMS mapping and data evaluation;** Martin Rittner¹; Steffen Bräkling¹; David Douglas²; Bence Paul³; ¹*TOFWERK, Gwatt (Thun), Switzerland*; ²*Elemental Scientific Lasers, Huntington, United Kingdom*; ³*Elemental Scientific Inc, Melbourne, Australia*

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- ThP 055 **Effects of Aromaticity on Petroleum Acid Fragmentation**; Esther Mbuna¹; Nathan Gard¹; Andrew Adam¹; Benjamin Bythell¹; ¹*Ohio University, Athens, OH*
- ThP 056 **Contribution of APCI-FTICR-MS for the molecular characterization of bio-oil from lignocellulosic biomass**; Charlotte Mase^{1,2,3}; Marie Hubert-Roux^{1,3}; Carlos Afonso^{1,3}; Pierre Giusti^{1,2,3}; ¹*University of Rouen, Mont Saint Aignan, France*; ²*TotalEnergies OneTech R&D, TotalEnergies Research & Technology, Gonfreville, France*; ³*International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harfleur, France*
- ThP 057 **Unraveling the Structural Secrets of Unique Compositions in Highly Complex Mixtures by High-Resolution Mass Spectrometry**; Jens Dreschmann¹; Wolfgang Schrader¹; ¹*Max-Planck-Institut für Kohlenforschung, Mülheim An Der Ruhr, Germany*
- ThP 058 **Applications of FT-ICR MS for the elucidation of oligomeric structures from thermochemical conversion of lignocellulosic biomass**; Evan Terrell^{1,2}; Melba Domes Denson²; Raiza Manrique Waldo³; Anthony Dufour⁴; Vincent Carre⁵; Frederic Aubriet⁵; Manuel Garcia-Perez²; ¹*USDA-ARS, Southern Regional Research Center, New Orleans, LA*; ²*Washington State University, Pullman, WA*; ³*Universidad Nacional de Colombia, Bogotá, Colombia*; ⁴*Universite de Lorraine, Nancy, France*; ⁵*Universite de Lorraine, Metz, France*
- ThP 059 **Methodology development for the monitoring of the use of Ionic Liquid in the removal of Naphthenic acids from Oil**; Sol Sauna Nety¹; Simiso Dube¹; Mathew M Nindi²; ¹*University of South Africa, Johannesburg, South Africa*; ²*UNISA, Florida Park, Roodepoort, South Africa*
- ThP 060 **Derivatized Carbazoles Dissociation Chemistry**; Dylan Carter¹; Jaya Paudel¹; Benjamin Bythell¹; ¹*Ohio University, Athens, OH*
- ThP 061 **Absorption mode Fourier Transform – Improved data quality for the FT-ICR MS analysis of extremely complex crude oil mixtures**; Alessandro Vetere¹; Wolfgang Schrader¹; ¹*Max-Planck-Institut für Kohlenforschung, Mülheim An Der Ruhr, Germany*
- ThP 062 **High throughput screening of mutant libraries using MALDI-ToF-MS analysis of microbial colonies for selecting fatty acid desaturase variants**; Kisurb Choe¹; Mike Jindra²; Susan Hubbard²; Blake Mirman¹; Brian F Pfeleger²; Jonathan V. Sweedler¹; ¹*University of Illinois at Urbana-Champaign, Urbana, IL*; ²*University of Wisconsin-Madison, Madison, WI*
- ThP 063 **Analysis of Neutral Organic Nitrogen Compound Present in Crude Oil Using Tandem Mass Spectrometry and Computational Chemistry**; Jaya Paudel¹; Lauren Davis¹; Dylan Carter¹; Benjamin Bythell¹; ¹*Ohio University, Athens, OH*
- ThP 064 **Characterization of pinewood-derived fast pyrolysis oil and its water-insoluble fraction with MRMS using ESI and APPI**; Hafiza Sajida Kousar¹; Timo Kekäläinen¹; Matthias Witt²; Janne Janis¹; ¹*University of Eastern Finland, Department of Chemistry, Joensuu, Finland*; ²*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*
- ThP 065 **Identification of Per and Polyfluorinated Alkyl Substances in Alternative Onsite Wastewater Treatment Systems by HRMS**; Rachel Smolinski¹; Meghan Oates²; Amith Maroli²; Arjun Venkatesan^{2,3}; Carrie A McDonough¹; ¹*Carnegie Mellon University, Pittsburgh, PA*; ²*New York State Center for Clean Water Technology, Stony Brook, NY*; ³*Stony Brook University, Stony Brook, NY*
- ThP 066 **Quantitation of Total PFAS including Trifluoroacetic Acid with Fluorine Nuclear Magnetic Resonance (19F-NMR)**; Dino Camdzic¹; Rebecca A. Dickman¹; Abigail S. Joyce²; Joshua S. Wallace¹; P. Lee Ferguson²; Diana S. Aga¹; ¹*University at Buffalo, Buffalo, NY*; ²*Duke University, Durham, NC*
- ThP 067 **Fast Screening of Perfluorinated Compounds Using Desalting Paper Spray Ionization Mass Spectrometry (DPSI-MS) Method**; Md. Tanim-AI Hassan¹; Praneeth Ivan Joel Fnu¹; Yongling Ai¹; Francis J. Osonga¹; Omowunmi A. Sadiq¹; Mengyan Li¹; Hao Chen¹; ¹*New Jersey Institute of Technology, Newark, NJ*
- ThP 068 **Analysis of Ultra-Short Through Medium Chain Length PFAS in Ground and Industrial Water by Multimode Chromatography-Mass Spectrometry**; Tanya Napolitano¹; Zijie Beryl Xia²; Alexander Schrum¹; Ronald Benson¹; ¹*Resonac America, Inc., New York, New York*; ²*Claros Technologies, Minneapolis, MN*
- ThP 069 **Identifying specific chemicals in aerosol particulate matter from various sources using mass spectrometry and artificial neural network analysis**; Geondo Park¹; Seungwoo Son¹; Yonghyeon Yim²; Sunghwan Kim^{1,3}; ¹*Department of Chemistry, Kyungpook National University, Daegu, South Korea*; ²*Korea Research Institute of Standards and Science (KRISS), Daejeon, South Korea*; ³*Mass Spectrometry Converging Research Center and Green-Nano Materials Research Center, Daegu, South Korea*
- ThP 070 **PFAS in Alligators of North Carolina's Cape Fear River: Assessing Spatial and Temporal Trends from 2018 to 2022**; Anna K. Boatman¹; Kylie D. Rock²; Scott M. Belcher²; Erin S Baker¹; ¹*University of North Carolina at Chapel Hill, Chapel Hill, North Carolina*; ²*North Carolina State University, Raleigh, NC*
- ThP 071 **Analysis of Targeted and Non-targeted Dye and Emerging Contaminants in the Kali-Loji River, Indonesia, Using UPLC-FT-ICR-MS**; Rafiqul Alam¹; Dede Heri Yuli Yanto²; Sunghwan Kim^{3,4}; ¹*Kyungpook National University, Daegu, South Korea*; ²*Research Center for Applied Microbiology, National Research and Innovation Agency (BRIN), Bogor, Indonesia*; ³*Department of Chemistry, Kyungpook National University, Daegu, South Korea*; ⁴*Mass Spectrometry Converging Research Center and Green-Nano Materials Research Center, Daegu, South Korea*
- ThP 072 **Utilizing Ion Mobility to Enhance Targeted and Non-Targeted Analysis of PFAS from Environmental Samples Collected at a Ski Resort**; Sarah Dowd¹; Kari Organtini¹; Marian Twohig¹; Jean Carlan²; Frank Dorman^{1,2}; ¹*Waters Corporation, Milford, MA*; ²*Department of Chemistry, Dartmouth College, Hanover, NH*
- ThP 073 **Analysis of Per- and Poly-fluoroalkylated Substances (PFAS) Specified in EPA Method 1633 Using Triple Quadrupole LC-MS/MS**; Om k Shrestha¹; Ethan Hain¹; Kathleen Luo¹; Christopher Gilles¹; Evelyn Wang¹; Xiaomeng Xia¹; Robert English¹; Tiffany Liden¹; ¹*Shimadzu Scientific Instruments, Columbia, MD*
- ThP 074 **Extremely sensitive, real-time detection of PFAS in the gas phase**; Joel R. Kimmel¹; Abigail Koss¹; Carla Frege²; ¹*TOFWERK AG, Boulder, CO*; ²*Tofwerk AG, Thun, Switzerland*
- ThP 075 **A Comprehensive Workflow for PFAS Analysis in Wastewater with Extended EPA Draft Method 1633 List**; Ruoji Luo¹; Emily Parry¹; Matthew Giardina¹; Linfeng Wu¹; Patrick Batoon¹; Tarun Anumol¹; ¹*Agilent Technologies, Inc., Santa Clara, CA*
- ThP 076 **The Effect of Water Properties on the Adsorption of Microcystins and Nodularin-R from Aqueous Samples by Treated Corncobs**; Hasaruwani S Kiridena¹; Manjula M Kandage¹; Norman Peiffer²; Michal Marszewski¹; Dragan Isailovic¹; ¹*University of Toledo, Toledo, OH*; ²*The Andersons, Maumee, OH 43537*
- ThP 077 **Quantification of Microplastics and Nanoplastics in firefighter gear and the environment**; Tommy M Nguven¹; O. David Sparkman¹; Liang Xue¹; Harry Allen²; Terry Ramus³; ¹*University of The Pacific, Stockton, CA*; ²*U.S. Environmental Protection Agency, Signal Hill, CA*; ³*Diablo Analytical Inc., Antioch, CA*
- ThP 078 **Method development for the non-targeted analysis of complex environmental contaminations - understanding oxidation processes in soil**; Wolfgang

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- ThP 079 **Schrader¹; Ruoji Luo¹; Ilker Satilmis¹; ¹Max-Planck Institut für Kohlenforschung, Mülheim, Germany**
New Directions in wastewater-based epidemiology. Identification of small and large biomolecules as biomarkers of public health and industrial activities; Ruben Gil Solsona¹; Jessica Subirats¹; Montserrat Carrascal²; Pablo Gago Ferrero¹; Antoni Ginebreda¹; Damia Barcelo^{1,3}; ¹IDAIA-CSIC, Barcelona, Spain; ²Info Institut d'Investigacions Biomèdiques August Pi i Sunyer, Barcelona, Spain; ³Catalan Institute for Water Research (ICRA), Girona, Spain
- ThP 080 **Spatial and Temporal Distributions of Per- and Polyfluorinated Alkyl Substances (PFAS) in Galveston Bay, TX; Yina Liu¹; Michael Shields¹; Sangeetha Puthigai¹; Xiaolei Xu¹; Shari Yvon-Lewis¹; ¹Texas A&M University, College Station, TX**
- ThP 081 **Optimizing a method to quantify per- and polyfluoroalkyl substances (PFAS) in house dust, silicone wristbands and handwipes; Sharon Zhang¹; Courtney C. Carignan²; Taylor Hoxie¹; Heather M Stapleton¹; ¹Duke University, Durham, NC; ²Michigan State University, East Lansing, MI**
- ThP 082 **Untargeted PFAS Suspect Screening and Quantitation of Community Water Samples from North Carolina's Cape Fear River Basin; Rebecca A Weed¹; Jeffrey Enders¹; Grace Campbell¹; Katlyn May¹; ¹North Carolina State University, Raleigh, NC**
- ThP 083 **Identification of Novel Degradation Products of Microcystins using UHPLC/MS and Automated Annotation of Their MSn Spectra; Sharmila I Thenuwara¹; Nicholas J Peraino²; Judy A Westrick²; Dragan Isailovic¹; ¹University of Toledo, Toledo, OH; ²Wayne State University, Detroit, MI**
- ThP 084 **Non-Targeted Analysis of Emerging Per- and Polyfluoroalkyl Substances (PFAS) in Rainwater; Yubin Kim¹; Kyndal A. Pike^{1,2}; Donald Conley¹; Jameson Sprankle¹; Rebekah Gray¹; Christopher Alaimo³; Thomas Young³; Jennifer Faust¹; Paul L Edmiston¹; ¹College of Wooster, Wooster, OH; ²University of Wisconsin-Madison, Madison, WI; ³University of California, Davis, Davis, CA**
- ThP 085 **Untargeted Exposure Analysis of Lake Okeechobee Using SPE-UHPLC-HRMS; Jae Hwan Lee¹; Ellen Titus²; Krista McCoy²; Timothy J. Garrett¹; ¹University of Florida, Gainesville, FL; ²Florida Atlantic University Harbor Branch Oceanographics, Fort Pierce, FL**
- ThP 086 **Comparing a Dried Blood Spot Microfluidic Chip to Whole Blood Analyses for PFAS Detection and Quantitation in Field Studies; Gregory Kudzin¹; James N Dodds¹; Hannah Starnes²; Zach Mclean²; Scott M. Belcher²; Erin S Baker¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, NC; ²North Carolina State University, Raleigh, NC**
- ThP 087 **GC-MS method with reduced solvent consumption for PBDE quantification in revalorized polymers; Marc-Antoine Vaudreuil¹; Richard Silverwood²; Alexandra Furtos-Matei¹; ¹Université de Montréal, Montreal, QC; ²Lavergne Inc., Montreal, QC**
- ThP 088 **Direct filter desorption of environmentally relevant chemicals using multi-scheme chemical ionization (MION) mass spectrometry; Joon Mikkilä¹; Fariba Partovi^{1,2}; Jyri Mikkilä¹; Tuija Jokinen³; Neha Deot³; Mikko J Sipilä⁴; Aleksei Shcherbinin¹; Matti P Rissanen²; HJ Jost¹; ¹Karsa Ltd, Helsinki, Finland; ²Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; ³Climate and Atmosphere Research Center (CARE-C), The Cyprus Institute, Nikosia, Cyprus; ⁴Institute for Atmospheric and Earth System Research (INAR), University of Helsinki, Helsinki, Finland**
- ThP 089 **Trimethylation enhancement using diazomethane (TrEnDi) enables enhanced LCMS detection of glufosinate and 3-(methylphosphinico)propionic acid from canola samples; Christian A Rosales¹; Krysten L Sheedy¹; Karl V Wasslen¹; Jeffrey M Manthorpe¹; Jeffrey C Smith¹; ¹Carleton University, Ottawa, ON**
- ThP 090 **Streamlining HRMS data acquisition and interpretation for wastewater impact on water quality; Michael Thurman¹; Imma Ferrer¹; James S Pyke²; ¹University of Colorado, Boulder, CO; ²Agilent Technologies, Santa Clara, CA**
- ThP 091 **Quantification of the Herbicide 2,4-Dichlorophenoxyacetic acid and of Specific Organophosphorous and Synthetic Pyrethroid Insecticides by LC-MS/MS; Dickson Wambua; CDC, Atlanta, GA**
- ThP 092 **Determination of Multiclass Pharmaceuticals in Environmental Samples by Liquid Chromatography-Tandem Mass Spectro; Xiaou Wei^{1,2,3}; Yujie Ben³; Chunmiao Zheng^{3,4}; Zongwei Cai^{1,2}; ¹State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, China; ²Department of Chemistry, Hong Kong Baptist University, Hong Kong, China; ³State Environmental Protection Key Laboratory of Integrated Surface Water-Groundwater Pollution Control, School of Environmental Science and Engineering, Southern University of Science and Technology, Shenzhen, China; ⁴EIT Institute for Advanced Study, Ningbo, China**
- ThP 093 **Development of a high-resolution LC-MS/MS workflow combining multiples activation methods for the general screening of pesticides; Romain Giraud¹; Yves Leblanc²; Mircea Guna²; Gérard Hopfgartner¹; ¹LSMS, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; ²SCIEX, Concord, ON**
- ThP 094 **Residue dissipation and dietary risk assessment of cyantraniliprole, spinetoram, and flonicamid in celery (Apium graveolens) under field conditions by LC-MS/MS; Yeong-Jin Kim¹; Sung-Gil Choi¹; Young Sang Kwon¹; Deuk-Yeong Lee²; Jong-Su Seo¹; Jong-Hwan Kim¹; ¹Environmental Safety Assessment Center, Gyeongnam Branch Institute, Korea Institute of Toxicology, Jinju, South Korea; ²Residue Chemical Assessment Division, Agro-Food Safety and Crop Protection Department, National Institute of Agricultural Sciences, Wanju, South Korea**
- ThP 095 **Water quality determination: a myriad of analysis simplified; Marcos Pudenzi¹; Luis Otavio Junqueira¹; ¹Shimadzu do Brasil LTDA, Barueri, Brazil**
- ThP 096 **Determination of multiresidue pesticides in Arabian Dates using LC and GC Triple Quadrupole Mass Spectrometry; Tuna Oncu¹; Orhan Papak¹; ¹Shimadzu Middle East and Africa FZE Istanbul, Istanbul, Turkey**
- ThP 097 **Measuring Antibiotics in Shoal Creek using Liquid Chromatography Mass Spectrometry during the COVID Pandemic; Cheyenne D Copling¹; Jacob Smith²; Katherine Maloof²; Jacob Pierson²; Hannah Konschak²; Leslie Kupferle²; Adam Sullivan²; Megan Davis²; Chloe Pancake²; Samuel Bickford²; Robert Dixon²; Kevin R Tucker²; ¹Southern Illinois University of Edwardsville, White/Caucasian, IL; ²Southern Illinois University Edwardsville, Edwardsville, IL**
- ThP 098 **PESTICIDES RESIDUE PRE-SCREENING USING KARSA MION INLET COUPLED TO ORBITRAP MASS SPECTROMETER WITH SELECTIVE CHEMICAL IONIZATION; Fariba Partovi^{1,2}; Joon Mikkilä²; Jussi Kontro²; Jyri Mikkilä²; Nasib Naseri²; Aleksei Shcherbinin²; Paxton Juuti²; Suvi Ojanperä³; Matti Rissanen^{4,5}; ¹Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; ²Karsa Ltd., Helsinki, Finland; ³Finnish Customs, Helsinki, Finland; ⁴Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; ⁵Department of Chemistry, University of Helsinki, Helsinki, Finland**
- ThP 099 **A Highly sensitive method for the determination of carbamates in water as per ASTM D-7645 by LCMS-8045; Shailesh Sadashiv Damale¹; Jessin Mathai¹; Kumar**

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- ThP 100 **Raju¹; Rajendra Makhama¹; Atul Narkar¹; ¹Shimadzu Middle East & Africa FZE, Dubai, United Arab Emirates**
Rapid low-cost testing of urine for unknown pesticide variants; Alexey Melnik^{1,2}; Olusola Onawoga²; David Chick²; Silverio Iacono^{2,3}; Alexander Aksenov^{2,4}; ¹University of Connecticut, Storrs, CT; ²Arome Science Inc., Farmington, CT; ³TomTec, Hamden, CT; ⁴University of Connecticut, Storrs, CT
- ThP 101 **Impact of Using 1.5 mm Column ID and Various Stationary Phases on LC/MS Pesticide Screening Analysis; Stephanie Schuster¹; Peter Pellegrinelli¹; Conner W. McHale¹; Benjamin Libert¹; Taylor Harmon¹; ¹Advanced Materials Technology, Inc., Wilmington, DE**
- ThP 102 **FluoroMatch 3.0 – Automated PFAS Non-Targeted Analysis and Visualizations Applied to Mammalian Biofluids; Michael Kummer¹; Nandarani Abril¹; Emily Parri²; Sheng Liu³; Carrie A McDonough⁴; David Dukes⁵; David Godri⁶; Elizabeth Z. Lin³; Emma E Rennie²; Jeremy Koelmel³; Krystal JG Pollitt³; ¹Innovative Omics, Sarasota, FL; ²Agilent Technologies, Santa Clara, CA; ³Yale University, New Haven, CT; ⁴Carnegie Mellon University, Pittsburgh, PA; ⁵Stony Brook University, Stony Brook, NY; ⁶3rd Floor Solutions, Toronto, Ontario**
- ThP 103 **HRMS-based Exposomics for Evaluating Embryonic Exposure and Cross-Placental Transfer of Xenobiotics; Max L Feuerstein^{1,2}; Tina Buerki-Thurnherr³; Benedikt Warth^{1,2}; ¹University of Vienna, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Währinger Straße 38, 1090, Vienna, Austria; ²Exposome Austria, Research Infrastructure and National EIRENE Hub, Vienna, Austria; ³Empa, Swiss Federal Laboratories for Materials Science and Technology, 9014 St. Gallen, Switzerland**
- ThP 104 **Generating MassBank-ready files from accurate mass library spectra: a proof-of-concept study; Andrew McEachran¹; Tristan Chutkan¹; Alex Chao²; Gregory Janesch³; Elin Ulrich²; Jon Sobus²; Antony Williams²; ¹Agilent Technologies, Santa Clara, CA; ²Chemical Characterization and Exposure Division, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, NC; ³ORAU Student Services Contractor to Center for Computational Toxicology and Exposure, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, NC**
- ThP 105 **Urinary DNA adductomics – a non-invasive, untargeted approach for the assessment of exposome-associated health risks; Carolina Möller¹; Alexandra Keidel²; Jazmine Virzi¹; Laura Deloso²; Yuan-Jhe Chang³; Mu-Rong Chao^{3,4}; Chiung-Wen Hu⁵; Marcus S. Cooke¹; ¹Oxidative Stress Group, Department of Molecular Biosciences, University of South Florida, Tampa, Florida 33620; ²Department of Chemistry, University of South Florida, Tampa, Florida 33620; ³Department of Occupational Safety and Health, Chung Shan Medical University, Taichung, Taiwan; ⁴Department of Occupational Medicine, Chung Shan Medical University Hospital, Taichung, Taiwan; ⁵Department of Public Health, Chung Shan Medical University, Taichung, Taiwan**
- ThP 106 **LC-MS workflow for large-scale profiling of mercapturic acids in human urine; Jin Y Chen¹; Zhengzhi Xie¹; Maleesha De Silva¹; Saurin R. Sutaria¹; Hong Gao¹; Sanjay Srivastava¹; Pawel Lorkiewicz¹; ¹University of Louisville, Louisville, KY**
- ThP 107 **Roles of HNOx and Carboxylic Acids in Thermal Stability of Nitroplasticizers; Kitmin Chen¹; Dali Yang¹; Zheng-hua Li¹; Oana C. Marina¹; Alexander S. Edgar¹; ¹Los Alamos National Laboratory, Los Alamos, NM**
- ThP 108 **Exposome-Wide Mapping of Circulating Caffeine Metabolites in Large Prospective Cohort Reveals Biochemical Links between Caffeine Exposure and Parkinson's Disease Risks; Yunjia Lai¹; Yujia Zhao²; Douglas I. Walker³; Christina M. Lill^{4,5}; Bastiaan R. Bloem⁶; Sirwan K.L. Darweesh⁶; Susan Peters²; Roel Vermeulen^{2,7}; Gary W. Miller¹; ¹Department of Environmental Health Sciences, Mailman School of Public Health, Columbia University, New York City, NY; ²Institute for Risk Assessment Sciences, Utrecht University, Utrecht, Netherlands; ³Department of Environmental Health, Rollins School of Public Health, Emory University, Atlanta, GA; ⁴Institute of Epidemiology and Social Medicine, University of Münster, Münster, Germany; ⁵School of Public Health, Imperial College London, London, United Kingdom; ⁶Radboud University Medical Center; Donders Institute for Brain, Cognition and Behaviour; Department of Neurology; Center of Expertise for Parkinson & Movement Disorders, Nijmegen, Netherlands; ⁷University Medical Centre Utrecht, Utrecht, Netherlands**
- ThP 109 **Wristband Personal Passive Samplers and Suspect Screening Methods Highlight Gender Disparities in Chemical Exposures; Nicholas Herkert¹; Jessica L Levasseur¹; Kate Hoffman¹; Gordon Getzinger²; P. Lee Ferguson²; Anna S Young³; Joseph G Allen³; Elizabeth Z Lin⁴; Krystal J Godri Pollitt⁴; Heather M Stapleton¹; ¹Nicholas School of the Environment, Duke University, Durham, NC; ²Department of Civil and Environmental Engineering, Duke University, Durham, NC; ³Department of Environmental Health, Harvard T.H. Chan School of Public Health, Boston, MA; ⁴Department of Environmental Health Sciences, Yale School of Public Health, New Haven, CT**
- ThP 110 **Quantitative Proteomic Analysis of Electronic-Cigarette Aerosol Exposed NOKSI cells: New Insights into the Pathways Involved; Mehari Weldemariam¹; Tao Ma²; Sarah L.J. Michel¹; Richard N. Dalby¹; Abraham Schneider²; Maureen A. Kane¹; ¹Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, Maryland; ²Department of Oncology and Diagnostic Sciences, University of Maryland School of Dentistry, Baltimore, Maryland**
- ThP 111 **MRM-profiling for detecting emerging contaminants in human biomonitoring: Application to Bisphenol A replacements; Jasmin Chovatiya¹; Ravikumar Jagani¹; Manish Arora¹; Syam S. Andra¹; ¹Institute for Exposomic Research, Department of Environmental Medicine and Public Health, Icahn School of Medicine at Mount Sinai, New York, NY**
- ThP 112 **Comprehensive Targeted Exposome Assay for Serum Samples; Jiamin Zheng¹; Lun Zhang¹; Mathew Johnson¹; Rupasri Mandal¹; David S. Wishart¹; ¹University of Alberta, Edmonton, AB**
- ThP 113 **Mapping the exposome of firefighters through the lens of mass spectrometry; Xiangping Lin¹; Xinyue Zhang¹; Basil Michael¹; Frank Wong¹; Mary Prunicki²; Kari Christine Nadeau²; Michael P. Snyder¹; ¹Department of Genetics, Stanford University, Stanford, CA; ²Sean N. Parker Center for Allergy and Asthma Research at Stanford University, Stanford, CA**
- ThP 114 **Structural elucidation of metabolites from bisphenol A analogs, BPB, BPAP and TBBPA, by high resolution tandem mass spectrometry; Said Matar^{1,2}; Ons Ousji^{2,3}; Lekha Sleno^{2,3}; ¹University of Quebec in Montreal, Montreal, QC; ²EcotoQ network on ecotoxicology research, Quebec, QC; ³University of Quebec in Montreal (UQAM), Chemistry department, Montreal, QC**
- ThP 115 **High-resolution mass spectrometry-based evaluation of limonene metabolites as biomarkers of greenness exposure; Zhengzhi Xie¹; Saurin R. Sutaria¹; Jin Y. Chen¹; Hong Gao¹; Daniel J. Conklin¹; Rachel J. Keith¹; Sanjay Srivastava¹; Aruni Bhatnagar¹; Pawel Lorkiewicz¹; ¹University of Louisville, Louisville, KY**
- ThP 116 **Utilizing Calibration Points to Replace Kovat's Indices to Confirm Tentatively Identified Compounds; Sarah T Pfahler^{1,2}; Robert Bradford^{1,2}; Jaehwan Lee²; Christin Duran²; John T Kelly³; Mitch Rubenstein³; ¹UES, DAYTON, Ohio; ²AFRL, 711th Human Performance Wing, DAYTON, Ohio; ³US AIR FORCE, DAYTON, OH**

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- ThP 117 **Liquid chromatographic retention time prediction models to secure and improve the feature annotation process in high-resolution mass spectrometry;** Julien Parinet¹; Yassine Makni²; Thierno Diallo²; Thierry Guérin¹; ¹ANSES, Maisons-Alfort, France; ²ANSES Maisons-Alfort, Maisons-Alfort, France
- ThP 118 **Effect of environmental exposome on early childhood atopic dermatitis;** Su Jung Kim¹; Mi Jeong Kim¹; Hyo Yeong Lee¹; Hyun Ju Yoo¹; ¹Asan Medical Center, Seoul, South Korea
- ThP 119 **Quality Control of Electronic-Cigarette Liquids by Helium-Plasma Ionization (HePI) Mass Spectrometry;** Kinan Khanzada¹; Logan Buddenbaum¹; Sihang Xu¹; Athula B. Attygalle¹; David Douce²; Steve Bajic²; ¹Stevens Institute of Technology, Hoboken, NJ; ²Waters Corporation, Milford, Milford, MA
- ThP 120 **Consumer Product Non-targeted Exposomics for Prospective Human Health;** Jenna Hua¹; Kristin A Favela²; William D Watson²; Jake A Janssen²; Michael J Harnett²; Heath A Spidle²; Jarod Grossman^{1,3}; ¹Million Marker Wellness, Inc., Berkeley, CA; ²Southwest Research Institute, San Antonio, TX; ³Agilent Technologies, Santa Clara, CA
- ThP 121 **Comparison of Targeted and Untargeted DNA Adductomics methods on an LC/qToF platform;** Nathan Montgomery¹; Corey Broeckling¹; ¹Colorado State University, Fort Collins, CO
- ThP 122 **Determination of Variance of Secondary Metabolites in Lettuces Grown Under Different Light Sources by FIMS and ANOVA-PCA;** Jianghao Sun¹; Mengliang Zhang²; Nicola Kubzdela¹; Yaguang Luo¹; James Harnly¹; Pei Chen¹; ¹USDA-ARS, Beltsville, MD; ²Middle Tennessee State University, Murfreesboro, TN
- ThP 123 **Nitrofurantol Metabolites and Chloramphenicol in Aquaculture Products using LC-MS/MS;** Brian Veach; Food and Drug Administration, Jefferson, AR
- ThP 124 **Determination of Benzophenone Derivatives in Bread in Taiwan by Solid-liquid Extraction-based UHPLC-MS/MS and Dietary Risk Assessment;** Yu-Fang Huang^{1,2}; Xuan-Rui Liu²; Chen-Ting Wu³; ¹Institute of Environmental and Occupational Health Sciences, National Yang Ming Chiao Tung University, Taipei, Taiwan; ²Department of Safety, Health and Environmental Engineering, National United University, Miaoli, Taiwan; ³Institute of Food Safety and Health Risk Assessment, National Yang-Ming Chiao Tung University, Taipei, Taiwan
- ThP 125 **Routine Quantitation of 17 Underivatized Amino Acids in Nutraceuticals and Animal Feed Using HPLC with a Fit-for-Purpose MSD Detector;** Greg Thompson¹; Sue D'Antonio²; Donna Payne³; Hui Zhao²; Mike Adams⁴; ¹Agilent Technologies, Wilmington, DE; ²Agilent Technologies, Wilmington, Delaware; ³AnalytEval, SMITHVILLE, TX; ⁴CWC Labs, Smithville, TX
- ThP 126 **Micro-QuEChERS coupled with UHPLC-MS/MS for Determination of Benzophenones and Parabens from Tea in Taiwan;** Chen-Ting Wu¹; Yu-Fang Huang²; ¹Institute of Food Safety and Health Risk Assessment, National Yang Ming Chiao Tung University, Taipei, Taiwan; ²Institute of Environmental and Occupational Health Sciences, National Yang Ming Chiao Tung University, Taipei, Taiwan
- ThP 127 **The application of a QTOF instrument to enable traceability of the origin of ginger;** Liuqing Zhao¹; Xiaogang Zhang²; Zong Yang³; Bingjie Liu³; Lihai Guo³; ¹SCIEX, Shanghai, China; ²SCIEX, Shanghai, China; ³SCIEX, Shanghai, China
- ThP 128 **Development of a Multi Analyte Method for the Screening of Dietary Supplement Products;** Christopher R. Beekman¹; Rahul Pawar¹; ¹U.S. Food and Drug Administration, College Park, MD
- ThP 129 **Simultaneous Quantification of South Korea representative Allergenic Foods with Optimized HPLC-MS/MS Approaches;** Min-Kyung Jun¹; Kyungdo Kim¹; Zee-Yong Park¹; Sangsuk Oh²; ¹School of Life Science, Gwangju Institute of Science and Technology, Cheomdangwagi123, Buk-gu, Gwangju, South Korea; ²Department of Food Science and Technology, College of Engineering, Ewha Womans University, Seoul, South Korea
- ThP 130 **Parallel-reaction monitoring detection of egg proteins for food allergen control: target peptide refinement and optimization;** Liyun Zhang¹; Philip Johnson¹; Melanie Downs¹; ¹Food Allergy Research and Resource Program, Department of Food Science and Technology, University of Nebraska-Lincoln, Lincoln, Nebraska, Lincoln, NE
- ThP 131 **Determination of authenticity of Manuka honey by MALDI-TOF mass spectrometry;** Simona Salivo¹; Tom K. Abban¹; Matthew E. Openshaw¹; Reda Hamour²; ¹Shimadzu, Manchester, UK, Manchester, United Kingdom; ²Shimadzu France, Marne La Vallee, France
- ThP 132 **Tracing the origins of red cabbage moss using a QTOF instrument for rapid nutrient identification;** Qing Liu¹; Liu qing Zhao²; Zong Yang³; Bing jie Liu⁴; Li hai Guo⁵; ¹SCIEX, nanchang, China; ²SCIEX, Shanghai, China; ³SCIEX, Shanghai, China; ⁴SCIEX, Beijing, China; ⁵SCIEX, China, Beijing, China
- ThP 133 **Quantitation of Polysaccharides in food using LC-MS/MS;** Jiani Jiang¹; Nikita P. Bacalzo, Jr. ¹; Carlito B. Lebrilla¹; ¹University of California, Davis, Davis, CA
- ThP 134 **Immunoaffinity Plastic Blade Spray Mass Spectrometry for Rapid Confirmatory Analysis of Food Contaminants1;** Ariadni Geballa-Koukoula¹; Arjen Gerssen¹; Marco Blokland¹; Michel Nielen^{1,2}; ¹Wageningen Food Safety Research (WFSR) part of Wageningen University & Research, Wageningen, Netherlands; ²Laboratory of Organic Chemistry, Wageningen University, Wageningen, Netherlands
- ThP 135 **Analysis of volatile compound in bovine milk samples using static headspace gas chromatography-mass spectrometry;** Dokyung Kwon¹; Hyojin Hwang¹; Jeongkwon Kim¹; ¹Department of Chemistry, Chungnam National University, Daejeon, South Korea
- ThP 136 **High-throughput UHPLC-MS/MS Analyses Optimizing the Flavor of Dairy Products;** Florian Utz¹; Andrea Spaccasassi¹; Timo D. Stark¹; Johanna Kreissl²; Caren Tanger³; Ulrich Kulozik³; Thomas F. Hofmann¹; Corinna Dawid¹; ¹Chair of Food Chemistry and Molecular Sensory Science, Technical University of Munich, Freising, Germany; ²Leibniz-Institute for Food Systems Biology at the Technical University of Munich, Freising, Germany; ³Chair of Food and Bioprocess Engineering, Technical University of Munich, Freising, Germany
- ThP 137 **Standardized metabolomics for the analysis of food enables confident and comparable chemical composition data;** Jessica Prenni¹; Jacqueline Chaparro¹; Corey Broeckling¹; Nathan Montgomery¹; Nichole Reisdorph²; Richard Reisdorph²; Cole Michael²; Katrina A Doenges²; Arpana Vaniya³; Oliver Fiehn³; Stacy D Sherrod⁴; Katrina L. Leaptrot⁴; Jody C. May⁴; John A. McLean⁴; Chi-Ming Chien⁵; Tracy Shafizadeh⁵; Steve Watkins⁵; ¹Colorado State University, Fort Collins, CO; ²University of Colorado Anschutz, Denver, CO; ³University of California Davis, Davis, CA; ⁴Vanderbilt University, Nashville, TN; ⁵Verso Biosciences, San Francisco, CA
- ThP 138 **Rapid Authentication of Red Wine by MALDI-MS Combined with DART-MS;** Xuewei Lin¹; Hao Wu²; Gefei Huang¹; Qian Wu¹; Zhongping Yao¹; ¹The Hong Kong Polytechnic University, Kowloon, Hong Kong; ²Xiamen University, Xiamen, China
- ThP 139 **Comprehensive analysis of functional ingredients using LC-MS/MS;** Kazuya Katada^{1,2}; Mami Okamoto¹; Jun Watanabe¹; Atsuhiko Toyama¹; Mari Maeda-Yamamoto^{2,3}; ¹Shimadzu Corporation, Kyoto, Japan; ²Self Care Food Council, Chiyoda-Ku, Japan; ³National Agriculture and Food Research Organization, Tsukuba, Japan
- ThP 140 **Retrospective screening of unknown emerging contaminants in tea using LC-HRMS;** Gui-Ru Xie¹; HONG-JHANG Chen²; ¹Health and Nutrition, SGS Taiwan

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- Ltd, New Taipei City, Taiwan; ²Institute of Food Science and Technology, National Taiwan University, Taipei, Taiwan*
- ThP 141 **Rapid detection of natural plant toxins using probe ESI unit combined with quadrupole time-of-flight mass spectrometer;** Tetsuo Iida¹; Kaoru Nakagawa¹; Manami Kobayashi²; ¹*Shimadzu Corporation, Kyoto-city, Japan;* ²*Shimadzu Corporation, Kawasaki-city, Japan*
- ThP 142 **When is Enough Actually Enough--How Does the Number of Replicates Influence the Quality of Non-Targeted Analysis Results?;** Karen E. Butler¹; Erica Bakota²; Christine M. Fisher³; Brian Ng³; Ann M. Knolhoff³; ¹*Joint Institute for Food Safety and Applied Nutrition, College Park, MD;* ²*Office of Regulatory Affairs, U.S. Food and Drug Administration, Lenexa, KS;* ³*Center for Food Safety and Applied Nutrition, U.S. Food and Drug Administration, College Park, MD*
- ThP 143 **Comparison of aroma profiles from different grades of black tea using a non-target metabolomics-approach;** Dave Bowman¹; Daniel Lukas¹; Paul M. Zelisko¹; Wendy E Ward¹; ¹*Brock University, St Catharines, ON*
- ThP 144 **Profiling of volatile ester isomers emitted from apple fruits by atmospheric pressure corona discharge ionization mass spectrometry;** Kanako Sekimoto¹; Yuto Nishikido¹; Toshio Hanada²; Kazuhisa Uchiyama³; Katsuhiko Shiratake⁴; ¹*Yokohama City Univ., Yokohama, Japan;* ²*National Agriculture and Food Research Organization, Morioka, Japan;* ³*Tokai Technology Center, Seto, Japan;* ⁴*Nagoya University, Nagoya, Japan*
- ThP 145 **Classification of Poultry Meat Cuts Based on the Approach of Untargeted Lipidomic Analysis and Advanced Chemometrics;** Ilias Tzavellas¹; Ioannis Martakos¹; Marilena Dasenaki¹; Ioannis Skoufos²; Athina Tzora²; Evagelos Gikas¹; Kevin Stup³; Carsten Baessmann⁴; Nikolaos S. Thomaidis¹; ¹*National and Kapodistrian University of Athens, Athens, Greece;* ²*University of Ioannina, School of Agriculture, Arta, Greece;* ³*Bruker Daltonics, Billerica, MA;* ⁴*Bruker Daltonics GmbH & Co. KG, Bremen, Germany*
- ThP 146 **Evolution of malt, hop and fermentation-derived flavor compounds throughout the brewing of a single malt, single hop (SMaSH) ale;** Christine A. Hughey¹; Amanda R Cicali¹; Angelina V Lo Presti¹; Lynn E Marsh¹; Ashleigh E Outhous¹; Leighann R Weber¹; Steve Harper¹; Samuel A Morton¹; ¹*James Madison University, Harrisonburg, VA*
- ThP 147 **Untargeted 4D Lipidomics combined with Chemometrics, as a reliable tool for the classification of pork meat cuts;** Ioannis Martakos¹; Ilias Tzavellas¹; Marilena Dasenaki¹; Ioannis Skoufos²; Athina Tzora²; Charalampos Proestos¹; Brian Teeter³; Carsten Baessmann⁴; Nikolaos S. Thomaidis¹; ¹*National and Kapodistrian University of Athens, Athens, Greece;* ²*University of Ioannina, School of Agriculture, Arta, Greece;* ³*Bruker Daltonics, Billerica, MA;* ⁴*Bruker Daltonics GmbH & Co. KG, Bremen, Germany*
- ThP 148 **Experimental and computational studies of the intrinsic reactivity of [O=U≡CH]⁺, [U-H]⁺, and U⁺;** Justin Terhorst¹; Samuel Lenze²; Michael Van Stipdonk²; ¹*Duquesne University, Jefferson Hills, PA;* ²*Duquesne University, Pittsburgh, PA*
- ThP 149 **Investigating the unimolecular dissociation of representative protonated terpenes and terpenoids;** Edgar White Buenger¹; Paul M. Mayer¹; ¹*University of Ottawa, Ottawa, ON*
- ThP 150 **Dissociation Chemistry of Substituted Indolines;** Lauren Elizabeth Davis¹; Esther Mbuna¹; Benjamin Bythell¹; ¹*Ohio University, Athens, OH*
- ThP 151 **Revisiting the Fragmentation Mechanism of Catechin Isomers;** Kuok-Fai Li¹; Pai-Chi Syue¹; Kuo-Lung Ku¹; ¹*National Chiayi University, Chiayi City, Taiwan*
- ThP 152 **Time-Resolved Collision Cross Section Measurements of Collision-Activated Gas-Phase Host-Guest Complexes;** Noah J Mismash¹; Savannah R Porter¹; Andrew J Arslanian^{1,2}; Bryce J Davis¹; Tanner Taylor¹; David V Dearden¹; ¹*Brigham Young University, Provo, UT;* ²*The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH*
- ThP 153 **Digital-Quadrupole Isolation of Native Protein Ions Allows for Interrogation of their Sequence and Structure with Electron Capture Dissociation;** Carter Lantz¹; Robert Schrader¹; Mirabel Sun¹; Joseph Meeuwssen²; Jared Shaw²; Joseph Beckman²; David Russell¹; ¹*Texas A&M Chemistry, College Station, TX;* ²*e-MSion, Corvallis, OR*
- ThP 154 **Leveraging ion-ion and ion-photon reactions to improve the sequencing of proteins carrying multiple disulfide bonds: the human albumin case study;** Linda Lieu¹; Joshua Hinkle²; John E.P. Syka²; Luca Fornelli^{1,3}; ¹*Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK;* ²*ThermoFisher Scientific, San Jose, CA;* ³*Department of Biology, University of Oklahoma, Norman, OK*
- ThP 155 **Design and Testing of a Hybrid Hyperthermal Atom-Ion Source for Ion Activation-Dissociation of Trapped Ions;** Dimitris Papanastasiou¹; Athanasios Smyrnakis¹; Alexandros Lekkas¹; Mariangela Kosmopoulou¹; ¹*Fasmatech, NCSR Demokritos, Athens, Greece*
- ThP 156 **Unexpected Gas-Phase Nitrogen-Oxygen Smiles Rearrangement: Collision-induced Dissociation of Deprotonated 2-(N-Methylanylino)ethanol and Morpholinylbenzoic Acid Derivatives;** Yuxue Liang¹; Yamil Simón-Manso²; Pedatsur Neta²; Xiaoyu Yang²; Yi Liu¹; Tallat Bukhari²; Stephen E. Stein²; ¹*National Institute of Standards and Technology, Gaithersburg, MD;* ²*National Institute of Standards and Technology, Gaithersburg, MD*
- ThP 157 **Exploration of UVPD fragmentation trends of peptides generated by MALDI;** Sean D Dunham¹; Erin H. Seeley¹; Jennifer S. Brodbelt¹; ¹*University of Texas at Austin, Austin, TX*
- ThP 158 **Operation of Simple SID Devices using Two or Three Voltages;** Andrew J Arslanian¹; Leon (Yu-Fu) Lin¹; Arpad Somogyi¹; Vicki H Wysocki¹; ¹*The Ohio State University, Columbus, OH*
- ThP 159 **Evaluation of Surface Induced Dissociation as a Higher Energy Approach to Gas-Phase Unfolding and Development of "Complex-Down" Gas Phase Unfolding;** Varun Gadkari¹; Rowan Matney¹; ¹*University of Minnesota, Twin Cities, Minneapolis, MN*
- ThP 160 **Investigating Vibrational Heat Capacities of Gas-Phase Biomolecular Ions for Use in Determining Ion Thermochemistry;** Lawren R. Paris¹; James S. Prell¹; ¹*University of Oregon, Department of Chemistry and Biochemistry, Eugene, OR*
- ThP 161 **Proton Affinities of Pepecolic Acid Containing Dipeptides from the Extended Kinetic Method;** J.C. Poutsma¹; Trinh Ton¹; Miko Miwa¹; Laurel Nicks¹; Katarina Faben¹; Mark Velasquez²; Mark Warren²; Jennifer Poutsma²; ¹*College of William & Mary, Williamsburg, VA;* ²*Old Dominion University, Norfolk, VA*
- ThP 162 **World building of a true instrument-independent database for product ion spectra in non-resonant mode be a chimera?;** Amandine Hueber¹; Annelaure Damont²; Hanna Kulyk³; Martin Green⁴; Ekaterina Darii⁵; Edith Nicol⁶; Sophie Liuu¹; Denis Lesage⁷; Yves Gimbert^{7,8}; Alain Perret⁵; Gwenaëlle LAVISON-BOMPARD⁹; Yacine Nia¹; Olivier Firmesse¹; Jacques Antoine Hennekinne¹; François Fenaille²; Christophe Junot²; Justine Bertrand-Michel¹⁰; Nicolas Cenac¹¹; Jean-Claude Tabet^{2,7,12}; ¹*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;* ²*CEA-INRA, Laboratoire Innovations en Spectrométrie de Masse pour la Santé (LI-MS), DRF / Institut Joliot / DMTS / SPI, MetaboHUB, CEA Saclay - Université Paris Saclay, Gif sur Yvette, France;* ³*Plateforme MetaboHUB-MetaToul - FluxoMet, Toulouse,*

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- France; ⁴Waters Corporation, Wilmslow, United Kingdom; ⁵Génomique métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry, France; ⁶Laboratoire de Chimie Moléculaire, CNRS – IP Paris, Ecole polytechnique, Palaiseau, France; ⁷IPCM - Sorbonne Université, UMR CNRS 8232, Paris, France; ⁸Département de chimie Moléculaire, UMR CNRS 5250, Université Grenoble Alpes, Grenoble, France; ⁹Pesticides and Marine Biotoxins unit (PBM), Laboratory for Food Safety, French Agency for Food, Environmental and Occupational Health & Safety (ANSES), Université Paris-Est, Maisons-Alfort, France; ¹⁰I2MC, Université de Toulouse, Inserm, MetaboHub, Toulouse, France; ¹¹IRSD, Université de Toulouse, INSERM, INRA, INP ENVT, Université de Toulouse 3 Paul Sabatier, Toulouse, France; ¹²Emeritus, Morangis, France
- ThP 163 **Gas-phase fragmentation of symmetric and asymmetric viologen-based host-guest complexes;** Daniel M Hristov¹; Hugo Y. Samayoa-Oviedo¹; Julia Laskin¹; ¹Purdue University, WEST LAFAYETTE, IN
- ThP 164 **Reactions of [UFXC2H]⁺(X=F, Cl, Br) with H₂O: Competition between the loss of C₂H₂ and HX;** Samuel J Lenze¹; Michael Van Stipdonk¹; Justin Terhorst¹; ¹Duquesne University, Pittsburgh
- ThP 165 **Gas-phase dissociation and thermal decomposition of mono- and di-cation ionic liquids;** Taofiq O Abdurraheem¹; Amanda Patrick¹; ¹Mississippi state university, Starkville, MS
- ThP 166 **Fimsbactin: an Ongoing Theoretical Study of bonding to FellII Forming Complexes;** Daryl Giblin¹; Michael L. Gross²; Timothy Wencewicz³; ¹Washington University, St Louis, MO; ²Washington University in St. Louis, St Louis, MO; ³Washington university in St louis, St Louis, MO
- ThP 167 **Peptide Chain Extension and Chiral Preference Mediated by Oxazolone Intermediate in Aqueous Microdroplets;** Lingqi Qiu¹; R. Graham Cooks¹; ¹Purdue University, WEST LAFAYETTE, IN
- ThP 168 **Spontaneous Prebiotic Condensation Reactions in Impinging Streams of Aqueous Microdroplets;** Dylan T. Holden¹; Nicolas M. Morato¹; Myles Q. Edwards¹; Lingqi Qiu¹; R. Graham Cooks¹; ¹Purdue University Department of Chemistry, West Lafayette, IN
- ThP 169 **A Multidimensional Approach to Probing the Binding Affinities of Poly(Lysine) and Poly(Styrene Sulfonate) Polyelectrolyte Complexes;** Calum Bochenek¹; Addie Keating¹; Chrys Wesdemiotis¹; ¹The University of Akron, Akron, OH
- ThP 170 **Gas-phase Acidity of D/L-Cysteine-Containing Oligopeptides by Computational and Mass Spectrometry Studies;** Shiyuan Wang¹; Yuntao Zhang²; Jianhua Ren²; ¹University of the Pacific, Stockton, CA; ²University of The Pacific, Stockton, CA
- ThP 171 **Automated Spectrum Annotation and Structure Disambiguation of Released N-linked Glycans;** Gary Wilson¹; Anastasia Chernykh²; Rebecah Kawahara²; St. John Skilton¹; Morten Thaysen-Andersen²; Marshall Bern¹; ¹Protein Metrics, LLC, Cupertino, CA; ²Macquarie University, Sydney, Australia
- ThP 172 **Absolute and relative quantification of bovine milk oligosaccharides using LC-MS based methods;** Yu Wang¹; Yu-Ping Huang¹; Sierra Durham¹; Daniela Barile¹; ¹UC Davis, Davis, CA
- ThP 173 **In-depth characterization of non-human sialic acid (Neu5Gc) in human serum using label-free ZIC-HILIC/MRM-MS;** Daum Lee^{1,2}; Nari Seo^{1,2}; Myung Jin Oh^{1,2}; Hyun Joo An^{1,2}; ¹Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; ²Asia Glycomics Reference Site, Chungnam National University, Daejeon, South Korea
- ThP 174 **Unusual free oligosaccharides found in human, bovine and caprine milk;** Weichien Weng¹; Chi-Kung Ni¹; ¹Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei City, Taiwan
- ThP 175 **Ultra-High-Throughput Microchip CE-MS Quantitative Glycomics Enabled by 18-plex Isobaric Multiplex Labeling Reagents for Carbonyl-Containing Compound (SUGAR) Tags;** Zicong Wang¹; Aditya Kulkarni²; Kate Yu²; Lingjun Li³; ¹University of Wisconsin-Madison, Madison, WI; ²908 Devices, Boston, MA; ³School of Pharmacy, University of Wisconsin-Madison, Madison, WI
- ThP 176 **Understanding the Structural Diversity of Immunogenic Glycans in Pig-to-Human Xenotransfusion using PGC-based LC/MS/MS;** Ji Eun Park^{1,2}; Myungjin Oh^{1,2}; Hyun Joo An^{1,2}; ¹Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; ²Asia-Pacific Glycomics Reference Site, Daejeon, South Korea
- ThP 177 **Absolute pharmacokinetics of heparin in primates by MRM;** Ke Xia; *Rensselaer Polytechnic Institute, Troy, NY*
- ThP 178 **Predicting Sialic Acid Content in N-Linked Glycans Using the Isotope Pattern of Chlorine;** Tana Palomino¹; David C Muddiman¹; ¹North Carolina State University, Raleigh, NC
- ThP 179 **LC-MS/MS Characterization of Glycans in Pig Sertoli Cells to Understand Complement System Behavior;** Andrew I. Bennett¹; Rachel L. Washburn²; Jannette M. Dufour²; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX; ²Texas Tech University Health Sciences Center, Lubbock, Texas
- ThP 180 **N-linked Glycan quantitation, is relative quantitation altered by label choice?;** Hoang Kim Ngan Thai¹; Ron Orlando¹; ¹University of Georgia - Complex Carbohydrate Research Center, Athens, GA
- ThP 181 **N-Glycome Profile of the Spike Protein S1: Systemic and Comparative Analysis of 11 variants of SARS-CoV-2;** Parisa Ahmadi¹; Cristian D Gutierrez Reyes¹; Sherifdeen Onigbinde¹; Akeem Adeyemi Sanni¹; Andrew I Bennett¹; Peilin Jiang¹; Oluwatosin Daramola¹; Mojgan Atashi¹; Vishal Sandilya¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock
- ThP 182 **De Novo Glycan Sequencing by PGC-nLC-ExD MS/MS and CID/HCD-ExD MS3 on an Omnitrap-Orbitrap Hybrid Instrument.;** Nadia Cherkassky¹; Chaoshuang Xia¹; Margaret Downs¹; Dimitris Papanastasiou²; Athanasios Smyrnakis²; Pengyu Hong³; Catherine E. Costello¹; Cheng Lin¹; ¹Boston University Chobanian and Avedisian School of Medicine, Boston, MA; ²Fasmatech, NCSR Demokritos, Athens, Greece; ³Brandeis University, Waltham, MA
- ThP 183 **Field-asymmetry ion mobility spectrometry to improve the separation and identification of released N-glycans;** Denis Morsa¹; Zoltan Szabo¹; Cornelia L Boeser¹; ¹Thermo Fisher Scientific, San Jose, CA
- ThP 184 **Evaluation of chromatographic columns and methods for the analysis of Mannose, Mannose Phosphates Mannose Nucleotides in plasma by LC-MS/MS;** Yashmitha Ravindra; *WuXi Apptec- Research Services Division, Cranbury, NJ*
- ThP 185 **LC-MS/MS Analysis of Heparan Sulfate and its components in cerebrospinal fluid, brain, liver and serum;** Lydia Lu; *WuXi Apptec- Research Services Division, Cranbury, NJ*
- ThP 186 **Evaluation of chromatographic columns and methods for the analysis sugars and sugar phosphates by LC-MS/MS;** Fatemeh Mousavi; *WuXi Apptec- Research Services Division, San Diego, CA*
- ThP 187 **Assessing N-glycan identification and quantitation from NISTmAb using ion mobility-mass spectrometry;** Jeffrey Enders¹; Taufika Islam Williams¹; Kenneth P Garrard¹; Steven Broome²; Rachel Harris²; Shahadat Reza²; David C Muddiman¹; ¹North Carolina State University, Raleigh, NC; ²MOBILion Systems, Inc, Chadds Ford, PA
- ThP 188 **Improved Hydrophilic Interaction Liquid Chromatography for LC/MS Analysis of Released N-Glycans;** Randall Robinson¹; Nandini Singh¹; Andrei Bordunov²; Steven Mast¹; Tom Rice¹; Aled Jones¹; Oscar

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- ThP 189 **Serum N-glycans analysis by LC-MS allows the prediction of patients' response to Vedolizumab treatment for Crohn's Disease**; Georgia Elgood-Hunt¹; Alex Adams²; Thomas Sénard¹; Richard Gardner¹; Wouter De Jonge³; Andrew Li Yim³; Alexandra Noble²; Jack Satsangi²; Vincent Joustra³; Geert Dhaens³; Daniel Spencer¹; ¹Ludger Ltd, Abingdon, United Kingdom; ²Oxford University, Experimental Medicine Division, Oxford, United Kingdom; ³Amsterdam University Medical Center, Inflammatory Bowel Disease Center, Amsterdam, Netherlands
- ThP 190 **Chemoenzymatic Synthesis of Sialylglycosphingosines using One-Pot MultiEnzyme (OPME)**; John McArthur¹; Pierce Carrouth¹; Katie Miller¹; Bailey Padgett¹; Dana Moore¹; L. Andrew Lee¹; ¹IMCS, Irmo, SC
- ThP 191 **D-Va: prediction and interpretation of intact N-glycopeptid tandem mass spectra by deep learning**; Zhewei Liang¹; Matthew P. Campbell²; Richard (DJ) Shipman¹; Monil Gandhi¹; Paul Aiyetan¹; Norton Kitagawa¹; Daniel Serie¹; ¹InterVenn Biosciences, South San Francisco, CA; ²InterVenn Biosciences, Melbourne, Australia
- ThP 192 **Allosteric regulation of proteasome function as established by H/D exchange mass spectrometry, cryo-EM, and molecular dynamics simulations**; Madison Turner¹; Samuel E. Hoff²; Adwaith B. Uday³; Algirdas Velyvis¹; Natalie Zeytuni³; Massimiliano Bonomi²; Siavash Vahidi¹; ¹University of Guelph, Guelph, ON; ²Institut Pasteur, Paris, France; ³McGill University, Montreal, Québec
- ThP 193 **Using Mass Spectrometry Techniques to Capture Mechanosensitivity in Cardiac Proteins**; Elena S Holden¹; Miranda Collier¹; Lucia Parolini¹; Dirk Aarts¹; Katja Gehmlich²; Justin LP Benesch¹; ¹University of Oxford, Oxford, United Kingdom; ²University of Birmingham, Birmingham, United Kingdom
- ThP 194 **Using membrane mimics (nanodiscs) to understand the structural and conformational dynamics of membrane proteins by TRESI-HDX-MS**; Vimanda Chow¹; Cristina Lento¹; Derek Wilson¹; ¹York University, Toronto, ON
- ThP 195 **Applications of PEPS-HDX-ESI-MS for measuring protein folding energies and folding/unfolding rates using a nonlinear two-state model fit**; Motolani Q Matthew^{1,2}; Rohana Liyanage^{1,2}; Shivakumar Sonnaila¹; Thallapuram Krishnaswamy S Kumar¹; Jackson Lay Jr. ^{1,2}; ¹UNIVERSITY OF ARKANSAS, FAYETTEVILLE, AR; ²Arkansas State-wide mass spectrometry facility, FAYETTEVILLE, AR
- ThP 196 **Establishing HDX-MS and other biophysical approaches to interrogate CC885 mediated GSPT1 degradation**; Shruti Navak¹; Paul Tawa¹; Cory Rice¹; Michael Eddins²; Thierry Fischmann¹; Li Xiao¹; Raphaelle Berger¹; David G. McLaren¹; Haihong Zhou¹; ¹Merck & Co., Inc., Kenilworth, New Jersey; ²Merck & Co., Inc., West Point, PA
- ThP 197 **Sensitivity Improvement of HDX-MS Method and its Applications in Therapeutic Protein Study: Epitope Mapping and Protein Interactions**; Xiao Pan; ¹Genentech, South San Francisco, CA
- ThP 198 **Differentiating Conformational Changes induced by Degraders & Non-degraders in BCL-6 and ERα using Hydrogen Deuterium Exchange Mass Spectrometry (HDX-MS)**; Ekaterina G. Devanova¹; Richard Y-C Huang^{1,2}; Robert Langish¹; Dalia Weiss³; Jinyi Zhu³; Andy Christoforou³; Isabella Tran³; Minerva Tran³; Veerabahu Shanmugasundaram⁴; Aaron Balog¹; David Weis¹; Petia Shipkova¹; Ingrid Wertz^{5,6}; ¹Bristol-Myers Squibb, Princeton, NJ; ²Janssen Research & Development, Spring House, PA; ³Bristol-Myers Squibb, San Diego, California; ⁴Bristol-Myers Squibb, Cambridge, MA; ⁵Lyterian Therapeutics, San Francisco, California; ⁶Bristol-Myers Squibb, Brisbane, CA
- ThP 199 **Probing the Effects of Hydrogen-Deuterium Exchange on Protein Stability in Solution and the Gas Phase**; Yousef Haidar¹; Lars Konermann²; ¹western university, London, ON; ²Western University, London, ON
- ThP 200 **Optimized Hydrogen/Deuterium Exchange Mass Spectrometry Analysis of SARS-CoV-2 Spike Ectodomain Shows Regional Differences in Conformational Dynamics**; Christopher A. Haynes¹; Theodore R. Keppel¹; Sarah Osman¹; Betlehem Mekonnen¹; Adrian R. Woolfitt¹; Yu Zhou¹; Dongxia Wang¹; John R. Barr¹; ¹Centers for Disease Control and Prevention, Atlanta, GA
- ThP 201 **Conformational Dynamics Analysis in SARS-CoV-2 Spike Variant Proteins Upon Interaction with Differentially Binding Antibodies Using Hydrogen/Deuterium Exchange Mass Spectrometry**; Theodore R. Keppel¹; Christopher A. Haynes¹; Adrian R. Woolfitt¹; Sarah H. Osman¹; Betlehem Mekonnen¹; Dongxia Wang¹; John R. Barr¹; ¹CDC, Atlanta, GA
- ThP 202 **Investigating the Influence of the Lipid Environment in Nanodiscs on the Dynamics and Insertion of Antimicrobial Pore-Forming Peptides**; Ron Dennis Siaden Ortega¹; Margot Di Cesare²; Jean-Michel Jault²; Cédric Orelle²; Etienne Meunier¹; Julien Marcoux¹; ¹IPBS Toulouse, Toulouse, France; ²Université de Lyon, Lyon, France
- ThP 203 **Epitope mapping of polyclonal antibodies in vaccine-elicited human serum**; Mulin Fang¹; Oliver Wu¹; Joel B. Langford¹; Kellye A. Cupp-Sutton¹; Kenneth Smith²; Kathleen Norris²; Judith A. James²; Si Wu¹; ¹University of Oklahoma, Norman, OK; ²Oklahoma Medical Research Foundation, Oklahoma City, OK
- ThP 204 **Hydrogen Deuterium Exchange Mass Spectrometry Reveals Protein Conformational Changes Upon N-terminal PEGylation**; Brent A Kochert¹; Ross Yang¹; Hongxia Wang¹; Hillary A. Schuessler¹; ¹Merck & Co., Inc., Kenilworth, New Jersey
- ThP 205 **HDX-MS and XL-MS analyses of antigen-IgG-FcγRIIIa interactions**; Yuki Yamaguchi¹; Natsumi Wakaizumi¹; Mine Irisa¹; Takahiro Maruno¹; Mari Shimada¹; Koya Shintani¹; Haruka Nishiumi¹; Rina Yogo^{2,3,4}; Saeko Yanaka^{2,3,4}; Daisuke Higo⁵; Tetsuo Torisu¹; Koichi Kato^{2,3,4}; Susumu Uchiyama^{1,2}; ¹Osaka University, Suita, Japan; ²Exploratory Research Center on Life and Living Systems (EXCELLS), National Institutes of Natural Sciences, Okazaki, Japan; ³Institute for Molecular Science (IMS), National Institutes of Natural Sciences, Okazaki, Japan; ⁴Nagoya City University, Nagoya, Japan; ⁵Thermo Fisher Scientific, Yokohama, Japan
- ThP 206 **Structural Mass Spectrometry on the Track of Neurodegenerative Diseases**; Petr Man^{1,2}; Zuzana Kalaninova^{1,2}; Sona Galuskova³; Tibor Mosko³; Michael Volny^{1,2}; Karel Holada³; Petr Novák^{1,2}; ¹BioCeV - Institute of Microbiology, Prague 4, Czech Republic; ²Charles University, Faculty of science, Prague, Czech Republic; ³Charles University, First Medical Faculty, Prague, Czech Republic
- ThP 207 **Transient structural dynamics during allosteric activation and inhibition of glycogen phosphorylase from non-equilibrium millisecond HDX-MS**; Monika Kish¹; Jonathan Phillips¹; ¹University of Exeter, Exeter, United Kingdom
- ThP 208 **The Effects of Kinetic Stabilizers on the Structural Dynamics of Amyloidogenic Immunoglobulin Light Chain Using Hydrogen Deuterium Exchange Mass Spectrometry**; Daniele Peterle¹; Nicholas L. Yan²; Elena S. Klimtchuk³; Thomas E. Wales¹; Olga Gursky³; Gareth J. Morgan³; Jeffery W. Kelly²; John R. Engen¹; ¹Department of Chemistry & Chemical Biology, Northeastern University, Boston, MA; ²Department of Chemistry, The Scripps Research Institute, La Jolla, CA; ³Amyloidosis Center,

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- Boston University Chobanian and Avedisian School of Medicine, Boston, MA*
- ThP 209 **Binding of Kif7 and Gli2 by hydrogen deuterium exchange mass spectrometry;** Bindu Y Srinivasu¹; Farah Haque^{2,3}; Radhika Subramanian^{2,3}; John R. Engen¹; ¹Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; ²Department of Molecular Biology, Massachusetts General Hospital, Boston, MA; ³Department of Genetics, Harvard Medical School, Boston, MA
- ThP 210 **Effect of Osmolytes on WNK Kinases by HDX;** Oladimeji Sunday Olaluwoye¹; Divyasri Damacharla²; Radha Akella³; John M Humphreys³; Darby Ball²; Elizabeth J Goldsmith⁴; Sheena D'arcy²; ¹The University of Texas at Dallas, Richardson, TX; ²The University of Texas at Dallas, Richardson, Texas; ³University of Texas Southwestern Medical Center, Dallas, TX; ⁴University of Texas Southwestern Medical Center, Dallas, Dallas, Texas, United States, Dallas, TX
- ThP 211 **The Acidic Domain of Asf1 Contributes to Binding Histones H3-H4 and Modulates Histone Acetyltransferase Rtt109;** Katayoun Morakabi¹; Noushin Akhavantab¹; Darby J Ball¹; Sheena D'arcy¹; ¹The University of Texas at Dallas, Richardson, Texas
- ThP 212 **Conformational Dynamics of TEM-type Extended Spectrum β -Lactamases as Revealed by Hydrogen/Deuterium Exchange Mass Spectrometry;** Tsz Fung Wong¹; Wai Po Kong¹; Pui Kin So¹; Yu Wai Chen¹; Zhongping Yao¹; ¹The Hong Kong Polytechnic University, Kowloon, Hong Kong
- ThP 213 **Ligand-induced conformational changes on β 1-Adrenergic Receptor coupled to miniGs mapped by Hydrogen-Deuterium Exchange Mass Spectrometry;** Joanna Toporowska¹; Parth Kapoor²; Jonathan Hopper²; Argyris Politis^{1,3}; ¹King's College London, London, United Kingdom; ²Mass Therapeutics, Oxford, United Kingdom; ³University of Manchester, Manchester, United Kingdom
- ThP 214 **Conformational dynamics of SARS-CoV-2 variant RBDs and their interactions with ACE2: Insights revealed by HDX-MS;** Dong Zhang¹; Tsz-Fung Wong¹; Pui-Kin So¹; Zhongping Yao¹; ¹The Hong Kong Polytechnic University, Kowloon, Hong Kong
- ThP 215 **Structural characterization of p97/VCP AAA+ ATPase via Hydrogen-Deuterium Exchange Mass-Spectrometry;** Ezgi Basturk¹; Baran Dingiloglu¹; Berfin Dogan¹; Gizem Dinler Doganay¹; ¹Istanbul Technical University, Istanbul, Turkey
- ThP 216 **Mapping Allosteric Regulation of Pyruvate Kinases by Native and Synthetic Ligands;** Evan Bonnard¹; Agnieszka Bogucka²; Marko Hyvönen²; Sheena D'arcy¹; ¹UT Dallas, Richardson, TX; ²University of Cambridge, Cambridge, United Kingdom
- ThP 217 **Tuning half-site reactivity: communication of chemically identical but dynamically different active sites over 100Å distance in Mo-dependent nitrogenase;** Monika Tokmina-Lukaszewska¹; Qi Huang²; Luke Berry³; Hayden Kallas⁴; John Peters⁵; Lance Seefeldt⁴; Simone Raugei²; Brian Bothner¹; ¹Montana State University, Bozeman, MT; ²PNNL, Richland, WA; ³MSU; BOZEMAN, MT, Bozeman, MT; ⁴Utah State University, Logan, UT; ⁵University of Oklahoma, Norman, OK
- ThP 218 **Heparin-induced changes in platelet factor IV conformation implicated in heparin-induced thrombocytopenia explored by H/D exchange;** Yi Du¹; Igor A Kaltashov¹; ¹University of Massachusetts-Amherst, Amherst, MA
- ThP 219 **Mechanism of complement cascade activation probed with HDX-MS;** Charles Mundorff¹; Michael Watson¹; Lauren Carter¹; Malika R Hale¹; Adian Valdez¹; David J Rawlings¹; Marion Pepper¹; Neil King¹; Miklos Guttman¹; ¹University of Washington, Seattle, WA
- ThP 220 **Determination of antibody epitopes against Sars-CoV2 antigens using Hydrogen Deuterium Exchange- Mass Spectrometry;** Ankit P Jain¹; Liu Xu¹; Filipp Frank¹; Wilbur Lam^{1,2,3,4}; Eric Ortlund¹; Blaine Roberts¹; ¹Emory School of Medicine, Emory University, Atlanta, GA; ²Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology & Emory University, Atlanta, GA; ³Aflac Cancer and Blood Disorders Center of Children's Healthcare of Atlanta, Atlanta, GA; ⁴Pediatric Technology Center, Children's Healthcare of Atlanta, Atlanta, GA
- ThP 221 **HDX-MS-guided drug discovery using the cancer driver Ras as a model system;** Evgeniy V. Petrotchenko¹; Roopa Thapar²; Edith Nagy²; Jason B. Cross²; Christoph H. Borchers^{1,3,4,5}; ¹Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; ²M.D. Anderson Cancer Center, Institute for Applied Cancer Science, Therapeutics Discovery Division, Houston, TX; ³Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; ⁴Division of Experimental Medicine, McGill University, Montreal, QC; ⁵Department of Pathology, McGill University, Montreal, QC
- ThP 222 **Integration of HDX and TIMS-q-ExD FT-ICR MS/MS for the Structural Characterization of Native Proteins;** Meiby Fernandez Rojas¹; Kevin Jeanne Dit Fouque²; Miguel Santos Fernandez²; Francisco Alberto Fernandez Lima²; ¹Florida International University, Miami, FL; ²Florida International University, Miami, FL
- ThP 223 **HDX-MS reveals novel aspects of PI3KC2b regulation by its extended N-terminus;** Gillian Leigh Dornan¹; Klara Haas¹; Volker Haucke¹; ¹Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany
- ThP 224 **HX-MS provides structural insights into the roles of mutations in structurally disordered regions of cancer-relevant proteins;** Malvina Papanastasiou¹; Amanda L Waterbury²; Hui Si Kwok²; Ceejay Lee²; Allyson M Freedy²; Cindy Su²; Will Hawkins¹; Andrew Reiter¹; Samuel M Hoening²; Michael E Vinyard²; Brian B Liau²; Steven A Carr¹; ¹Broad Institute, Cambridge, MA; ²Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA
- ThP 225 **Hydrogen/Deuterium Exchange of a Polyketide Synthase During Its Catalytic Cycle;** Josh Salem¹; Rebecca Taylor²; Kristina Hakansson²; ¹University of Michigan, Ann Arbor, MI; ²University of Michigan-Ann Arbor, Ann Arbor, MI
- ThP 226 **Mapping interactions of staph enterotoxin B in neutralizing serum;** Clint Vorauer¹; Camila Boniche-Alfaro²; Bettina Fries²; Mike Guttman¹; ¹University of Washington, Seattle, WA; ²Stony Brook University, Stony Brook, NY
- ThP 227 **Capsid-genome rearrangements drive asymmetric RNA egress and virus disassembly by integrative structural mass spectrometry and cryo-EM;** Ganesh S Anand¹; Varun Venkatakrisnan¹; Sean Braet¹; ¹The Pennsylvania State University, University Park, PA
- ThP 228 **Rapid and High-Throughput Screening of 3 Cannabinoids in Cell Culture Medium Using the Echo® MS system;** Pengyi Hou¹; Dandan Si¹; Zhimin Long²; Lihai Guo¹; ¹SCIEX, Beijing, China; ²SCIEX, Shanghai, China
- ThP 229 **SP3-enabled high coverage multiplexed cysteine chemoproteomics;** Flowreen Shikwana¹; Alexandra C. Turmon¹; Miranda Villanueva¹; Cindy Truong¹; Keriann Backus¹; ¹UCLA, Los Angeles, CA
- ThP 230 **The S-Trap for Clean and Robust Automated Sample Preparation in Bottom-Up Proteomics;** Stefan Loroch^{1,2}; John P Wilson²; ¹Medical Proteome-Center, Ruhr-University, Bochum, Germany; ²Protifi, LLC, Fairport, NY
- ThP 231 **High-throughput label-free opioid receptor binding assays using automated desorption electrospray ionization mass spectrometry (DESI-MS);** Yunfei Feng¹; Nicolas M. Morato¹; Kai-Hung Huang¹; R. Graham Cooks¹; ¹Purdue University, WEST LAFAYETTE, IN
- ThP 232 **Development of a high-throughput MALDI-TOF MS biochemical screen for inhibitors of an**

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- aminopeptidase; Leonie Mueller¹; Simon Peace²; Melanie Leveridge³; Matthias Trost¹; Rachel Peltier-Heap⁴; Maria Emilia Dueñas¹; ¹Newcastle University, Newcastle upon Tyne, United Kingdom; ²GSK, Medicinal Chemistry, Stevenage, United Kingdom; ³GSK, Screening, Profiling and Mechanistic Biology, Stevenage, United Kingdom; ⁴GSK, Discovery Analytical, Stevenage, United Kingdom
- ThP 233 **Automated Data Analysis and Robust Quality Control for Affinity Selection Mass Spectrometry**; Matthew Green¹; Juan Florez²; Malwina Michalak³; Stephan Steigeler²; Stephan Heyse²; ¹Genedata, Cambridge, United Kingdom; ²Genedata, Basel, Switzerland; ³Genedata, Munich, Germany
- ThP 234 **Untargeted LC-MS metabolomics screening of 500,000 serum samples identifies novel biomarkers for cancer, cardiovascular, and liver diseases**; Boris Sarvin¹; Mark Vernik¹; Avi Shoshan¹; Eldad Kepten¹; Carmel Shor¹; Ori Kronfeld¹; Avishai Gavish¹; Shira Shaham-Niv¹; Tomer Shlomi^{1,2}; ¹MetaSight Diagnostics LTD, Rehovot, Israel; ²Faculty of Biology and Computer Science, Technion—Israel Institute of Technology, Haifa, Israel
- ThP 235 **New Applications of High Throughput IR-MALDESI-MS for Lead Discovery**; Fan Pu¹; Andrew Radosevich¹; Omprakash Nacham¹; James Sawicki¹; Nari Talaty¹; Scott Ugrin¹; Sujatha Gopalakrishnan¹; Jon Williams¹; Nathaniel Eisen¹; ¹AbbVie Inc., North Chicago, IL
- ThP 236 **Acoustic Ejection Mass Spectrometry for Ultrahigh-Throughput Analysis of Pharmaceutical Targets**; Hang Hu¹; Ophelia Ukaegbu¹; Joseph Gouker¹; Stephanie Chun¹; Wai Ling Cheung-Lee¹; Karla Camacho Soto¹; Hsing-I Ho¹; Amanda Marie Makarewicz¹; Stephanie Galanie¹; Xijuan Wen²; David G. McLaren²; Kevin P. Bateman³; Chang Liu⁴; Thomas R. Covey⁴; Erik L. Regalado¹; Emmanuel Appiah-Amponsah¹; ¹Merck & Co., Inc., Rahway, NJ; ²Merck & Co., Inc., Kenilworth, NJ; ³Merck & Co., Inc., West Point, PA; ⁴SCIEX, Concord, ON
- ThP 237 **High throughput characterization of polyamide hydrolase activity using open port sampling interface mass spectrometry**; John F. Cahill¹; Vilmos Kertesz¹; Patricia Saint-Vincent¹; Hannah Valentino¹; Erin Druvfa¹; Joshua K. Michener¹; ¹Oak Ridge National Laboratory, Oak Ridge, TN
- ThP 238 **A rapid workflow for high-throughput FFPE-based proteomics**; Ganesh Pujari¹; Kiran Mangalaparthy¹; M. Cristine Charlesworth¹; Benjamin Madden¹; Amy Josephine French¹; Gunveen Sachdeva¹; Eugenio Daviso²; Ulrich Thomann²; Patrick McCarthy²; Sameer Vasantgadkar²; Deb Bhattacharyya²; Akhilesh Pandey¹; ¹Mayo Clinic, Rochester, Minnesota; ²Covaris, Lexington, MA
- ThP 239 **Building spectral libraries to enable large-scale quantitative proteomic studies in human plasma**; Jian Wang¹; Harendra Guturu¹; Yingxiang Huang¹; Seth Just¹; Shadi Ferdosi¹; Xiaoyan Zhao¹; Andrew Nichols¹; Lee S Cantrell¹; Alexey Stukalov¹; Iman Mohtashemi¹; Ting Huang¹; Lucy Williamson¹; Gabriel Castro¹; Eltaher Elgierari¹; Ryan W. Benz¹; Khatereh Motamedchaboki¹; Daniel Hornburg¹; Asim Siddiqui¹; Serafim Batzoglou¹; ¹Seer, Inc., Redwood City, CA
- ThP 240 **Rapid Characterization of Unpurified Biotherapeutics through Online Buffer Exchange**; Michael Poltash¹; Weijing Liu²; Elsa Gorre¹; Scott Kronewitter²; Rosa Viner²; Andrew Mahan¹; Hirsh Nanda¹; ¹Janssen Pharmaceuticals, Spring House, PA; ²Thermo Fisher Scientific, San Jose, California
- ThP 241 **High-throughput proteomics on a novel high-resolution accurate mass (HRAM) platform**; Tabiwang N. Arrey¹; Daniel Hermanson²; Jeff Op De Beeck³; Runsheng Zheng⁴; Xuefei Sun⁵; Paul Jacobs³; Nicolaie Eugen Damoc¹; Vlad Zabrouskov²; ¹Thermo Fisher Scientific, Bremen, Germany; ²Thermo Fisher Scientific, San Jose, California; ³Thermo Fisher Scientific - Belgium, Ghent, Belgium; ⁴Thermo Fisher Scientific, Germering, Germany; ⁵Thermo Fisher Scientific, Sunnyvale, CA
- ThP 242 **The development of Acoustic Ejection Mass Spectrometry as a high-throughput, label-free platform for cell-based profiling of metabolic processes**; Amy Burton¹; Justin T Munro²; Michelle Pemberton¹; Julie Quayle¹; Joseph Kozole²; Roland Annan²; ¹Discovery Analytical, Screening, Profiling, and Mechanistic Biology, GlaxoSmithKline, Stevenage, United Kingdom; ²Discovery Analytical, Screening, Profiling, and Mechanistic Biology, GlaxoSmithKline, Collegeville, PA
- ThP 243 **Integration of Desorption Electrospray Ionization and 2D-MS/MS for High Throughput Experimentation**; Eric T. Dziekonski¹; Thomas C. Sams¹; Lucas J. Szalwinski¹; L. Edwin Gonzalez¹; R. Graham Cooks¹; ¹Purdue University, WEST LAFAYETTE, IN
- ThP 244 **High-Throughput Mass Spectrometry Enables Rapid Genome Engineering**; Alessandra Paul; *Infinome Biosciences, San Bruno, CA*
- ThP 245 **iFishMass: a new software for high-throughput signal extraction of Direct Infusion Mass Spectrometry runs**; Carlos J Madrid-Aliste¹; Jennifer Aguilan¹; Simone Sidoli¹; ¹Albert Einstein College of Medicine, Bronx, NY
- ThP 246 **Ion pre-accumulation in bent flatplate boosts MS2 sensitivity and peptide identifications in an Orbitrap Exploris 480 mass spectrometer**; Florian Harking¹; Julia Kraegenbring²; Hamish Stewart²; Pedro Navarro²; Konstantin Ayzikov²; Dmitry Grinfeld²; Alexander Harder²; Alexander Makarov²; Jesper Velgaard Olsen¹; ¹NNF CENTER FOR PROTEIN RESEARCH, Copenhagen, Denmark; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- ThP 247 **Quantification of Terpenes with Rapid "Shotgun" APGC-IMS-MS**; Jeffrey Morre¹; Sam Bassett²; Claudia Maier²; Jan F. Stevens^{2,3}; ¹Oregon State University, Corvallis, OR; ²Oregon State University, Corvallis; ³Global Hemp Innovation Center, Corvallis, OR
- ThP 248 **Multi-omic Analyses Enabled by Microchip Capillary Electrophoresis and Trapped Ion Mobility Mass Spectrometry**; Zhan Gao¹; Melissa R. Pergande¹; Matthew S Fischer¹; Eli J Larson¹; Morgan Mann¹; Kevin M. Buck¹; Jake A Melby¹; Yanlong Zhu¹; Adi M Kulkarni²; J. Will Thompson²; Guillaume Tremintin³; Kate Yu²; Ying Ge¹; ¹University of Wisconsin-Madison, Madison, WI; ²908 Devices, Inc., Boston, MA; ³Bruker Daltonics, San Jose, CA
- ThP 249 **Operating the Orbitrap Platform in Data-Dependent Acquisition Mode: Electron Induced and Electron Capture Dissociation of BSA and HeLa Digests**; Mariangela Kosmopoulou¹; Athanasios Smyrnakis¹; George Alexivos¹; Dimitris Papanastasiou¹; ¹Fasmatech, NCSR Demokritos, Athens, Greece
- ThP 250 **High-throughput metabolic screening using neutron encoded 96-plex tags**; Michael R Armbruster¹; Scott F Grady¹; Christopher K Arnatt¹; James L Edwards¹; ¹Saint Louis University, St. Louis, MO
- ThP 251 **High-Depth Multiplexed Drug Profiling with the Orbitrap Ascend**; Steven R. Shuken¹; Graeme C. McAlister²; William D. Barshop²; Jesse D. Canterbury²; David Bergen²; Jingjing Huang²; Romain Huguet²; Joao A. Paulo¹; Amanda E Lee²; Vlad Zabrouskov²; Steven P Gygi¹; Qing Yu¹; ¹Department of Cell Biology, Harvard Medical School, Boston, MA; ²Thermo Fisher Scientific, San Jose, California
- ThP 252 **"Affinity-Selection Mass Spectrometry (MagMASS) for the Discovery of Inhibitors of the SARS-CoV-2 Papain-like Protease (PLpro)"**; Daniel D Simchuk¹; Andrew D. Mesecar²; Mackenzie E Chapman-Imhoff²; Richard Van Breenen³; ¹Oregon State University, Corvallis, OR; ²Purdue University, WEST LAFAYETTE, IN; ³Oregon State University, Corvallis
- ThP 253 **High-throughput bioanalysis of adenosine by LS-ILC-MS/MS platform**; Yuanqiang Su¹; Ke Song¹; Xiaotong Li¹; Xinxin Wen¹; Juezhu Fan¹; Cheng Chen¹; Zhiyu Li¹; Lili Xing¹; Yi Tao¹; Liang Shen¹; ¹WuXi AppTec, Shanghai, China

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- ThP 254 **Subcellular Resolution Biochemical Imaging Method Combining Electron Microscopy with Vacuum Electrospray Beams**; John Sentmanat¹; Peter A Kottke¹; Andrei G Fedorov¹; ¹*Georgia Institute of Technology, Atlanta, GA*
- ThP 255 **Hadamard transform AP-MALDI imagery with a digital micro-mirror array**; Jun J Hu; *Ningbo University, Ningbo, China*
- ThP 256 **Maximizing the Spatial Information of IR-MALDESI Mass Spectrometry Imaging of Zebrafish Using a Top-Hat Beam and Variable Step Size**; Alena N Joignant¹; David C Muddiman¹; ¹*FTMS Laboratory for Human Health Research, Department of Chemistry, Raleigh, NC*
- ThP 257 **Improvements in a Multi-Reflecting ToF Mass Spectrometer to Enhance Mass Spectrometry Imaging Specificity**; Emmanuelle Claude¹; William Johnson¹; Joel Keelor²; Emma Marsden-Edwards¹; Martin Palmer¹; ¹*Waters Corporation, Wilmslow, United Kingdom*; ²*Waters Corporation, Milford, MA*
- ThP 258 **Response Surface Methodology for Optimization of nano-DESI Imaging using Orbitrap Instruments**; Felix Friedrich¹; Ingela Lanekoff¹; ¹*Uppsala University, Uppsala, Sweden*
- ThP 259 **Development of ambient mass spectrometry imaging using laser ablation electrospray ionization separated by gas transportation for analyses of intracellular molecules**; Riku Hirota¹; Hisanao Hazama¹; Kunio Awazu²; ¹*Graduate School of Engineering, Osaka University, Suita, Japan*; ²*Global Center for Medical Engineering and Informatics, Osaka University, Suita, Japan*
- ThP 260 **fibTOF: Sensitive imaging of light elements at nanometer resolution**; Valentine Riedo-Grimaudo¹; Lex Pillatsch¹; James Whitby¹; Michael Grössl¹; Steffen Bräkling¹; ¹*Tofwerk AG, Thun, Switzerland*
- ThP 261 **Comprehensive Assessment of MALDI-2 IMS Performance on Human and Murine Tissues**; Kameron R Molloy^{1,2}; Madeline E Colley^{2,3}; Lukasz G Migas^{2,4}; Allison B Esselman^{1,2}; Martin Duffresne^{2,3}; Raf Van De Plas^{2,3,4}; Jeffrey M Spraggins^{1,2,3,5}; 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*
- ThP 262 **Picosecond Infrared Laser Desorption – Rapid Evaporative Ionisation Mass Spectrometry for Molecular Pathology and Imaging**; Daniel Simon^{1,2}; Ronan Battle²; Yuchen Xiang²; Stefania Maneta-Stavarakaki²; Lauren Ford²; Robert T Murray²; Josephine Bunch³; Zoltan Takats^{1,2}; ¹*Rosalind Franklin Institute, Harwell, Didcot, United Kingdom*; ²*Imperial College London, London, United Kingdom*; ³*National Physical Laboratory, Teddington, United Kingdom*
- ThP 263 **Coupling AP-SMALDI MS Imaging technology with Orbitrap Exploris MX mass detector**; Domenic Dreisbach¹; Carolin M Morawietz²; Karl Christian Schäfer¹; Kerstin Strupat³; Bernhard Spengler^{1,2}; ¹*Transmit GmbH, Giessen, Germany*; ²*Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Gießen, Germany*; ³*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*
- ThP 264 **In-capillary dielectric barrier discharge post-ionization for MALDI MSI of metabolites and lipids**; Sven Heiles^{1,2}; Bernhard Spengler³; Sabine Schulz³; Julian Schneemann³; Karl-Christian Schäfer⁴; ¹*Leibniz Institute for Analytical Sciences - ISAS - e.V., 44139 Dortmund, Germany*; ²*Faculty of Chemistry, University of Duisburg-Essen, 44139 Essen, Germany*; ³*Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Germany*; ⁴*TransMIT GmbH, Giessen, Germany*
- ThP 265 **HiPLEX-IHC MALDI Imaging of FFPE Kidney tissue at 5µm utilizing microGRID on timsTOF fleX MALDI-2**; Connor West¹; Joshua Fischer¹; Corinna Henkel²; Gargey B. Yagnik³; Mark Lim³; ¹*Bruker Scientific, LLC, Billerica, MA*; ²*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*; ³*AmberGen, Inc., Billerica, MA*
- ThP 266 **Dual-LIT Instrumentation for MS/MS Imaging and Single-Cell Lipidomics**; Zheng Ouyang¹; Xiangyu Gu Guo¹; Aojie Zhang¹; Zhijun Cai; Wenpeng Zhang¹; ¹*Tsinghua University, Department of Precision Instrument, Beijing, China*
- ThP 267 **Development of a High Throughput Microscope-Mode Secondary Ion Imaging Mass Spectrometer**; Elena Castellani^{1,2}; Yifeng Jia¹; Anya Eyres^{1,3}; Natasha Smith¹; Michael Burt¹; Josephine Bunch^{2,3}; Zoltan Takats^{2,4}; Mark Brouard¹; Felicia M Green²; ¹*University of Oxford, Dept. of Chemistry, Oxford, United Kingdom*; ²*Rosalind Franklin Institute, Harwell, Didcot, United Kingdom*; ³*National Physical Laboratory, Teddington, United Kingdom*; ⁴*Imperial College, London, London, United Kingdom*
- ThP 268 **High resolution MALDI imaging mass spectrometry of mouse fetuses to assess markers of neural tube defects after maternal opioid exposure**; Dustyn A Barnette¹; Richard Beger¹; Pravin R. Kaldhore¹; Joseph Hanig²; J. Edward Fisher²; Dan Mellon²; Grace Lee³; Amy Inselman¹; E. Ellen Jones¹; ¹*National Center for Toxicological Research, Jefferson, AR*; ²*Center for Drug Evaluation and Research, Silver Spring, MD*; ³*Elevor Therapeutics, Salt Lake City, UT*
- ThP 269 **Changes in spatial distribution of brain N-glycans in acute stress-induced mouse models using MALDI mass spectrometry imaging (MSI)**; Hyun Jun Jang¹; Hyecheon Kang¹; Boyoung Lee¹; ¹*Institute for Basic Science, Daejeon, South Korea*
- ThP 270 **Mass spectrometry imaging reveals lipidomic changes in skeletal muscles due to muscle hypertrophy**; Naoko GOTO-INOUE; *Nihon University, Fujisawa, Japan*
- ThP 271 **Traumatic brain injury and MSI-AP-MALDI: map of small metabolites in the different brain regions**; Angela Marika Siciliano¹; Laura Brunelli¹; Giulia De Simone¹; Aurelia Morabito¹; Francesca Pischiutta¹; Federico Moro¹; Elisa R. Zanier¹; Roberta Pastorelli¹; Enrico Davoli¹; ¹*Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy*
- ThP 272 **In situ lipidomics of Staphylococcus aureus bone infection using MALDI imaging mass spectrometry**; Christopher J Good^{1,2}; Casey E Butrico³; Elizabeth K Neumann^{1,4}; Madeline E Colley^{1,4}; Katherine N Gibson-Corley³; Lukasz G Migas⁵; Raf Van De Plas⁵; James E Cassat^{3,6,7,8}; Jeffrey M Spraggins^{1,2,4,9}; Richard M Caprioli^{1,2,4,10,11}; ¹*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*; ²*Department of Chemistry, Vanderbilt University, Nashville, TN*; ³*Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN*; ⁴*Department of Biochemistry, Vanderbilt University, Nashville, TN*; ⁵*Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands*; ⁶*Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN*; ⁷*Department of Biomedical Engineering, Vanderbilt University, Nashville, TN*; ⁸*Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University Medical Center, Nashville, TN*; ⁹*Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN*; ¹⁰*Department of Medicine, Vanderbilt University, Nashville, TN*; ¹¹*Department of Pharmacology, Vanderbilt University, Nashville, TN*
- ThP 273 **Quantifying Multiple Anti-tuberculosis Drugs in Infected Mouse Tissue by MALDI Mass Spectrometry Imaging**; Michael Tuck¹; Florent Grélard¹; Landry Blanc¹; Véronique Dartois²; Nicolas Desbenoit¹; ¹*Université de Bordeaux, Bordeaux, France*; ²*Hackensack Meridian Health Center for Discovery & Innovation, Nutley, NJ*

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- ThP 274 **Laser ablation inductively coupled plasma mass spectrometry imaging reveals how gold nanoparticle surface charge influences their distribution and excretion pathways;** Jeerapat Doungchawee¹; Laura J Castellanos¹; Kristen Sikora¹; Xianzhi Zhang¹; Yuanchang Liu¹; Vincent M. Rotello¹; Richard W. Vachet¹; ¹University of Massachusetts Amherst, Amherst, MA
- ThP 275 **Mass Spectrometry Imaging of Brain Fatty Acids and Behavioral Studies on Prenatal Cannabis Exposure and Omega-3 Fatty Acid Diet Supplementation;** Samantha L. Cousineau¹; Mohammed H. Sarikahya¹; Marta De Felice¹; Aleksandra Doktor¹; Steven R. Laviolette¹; Daniel B. Hardy¹; Ken K.-C. Yeung¹; ¹University of Western Ontario, London, ON
- ThP 276 **Spatiotemporal Profiling of the Lipidome, Proteome, and Phosphoproteome of PLK1 Inhibited Colorectal Cancer Spheroids;** Emily R. Sekera¹; Brian D. Fries¹; Amanda B. Hummon¹; ¹The Ohio State University, Columbus, OH
- ThP 277 **Visualizing the spatial distribution of flavonoids and phenolic acids in the tuber root of *Tetragonia hemsleyana* using AP-MALDI-MSI;** Junling Dun¹; Hongyuan Hao¹; Taohong Huang¹; Yan Lin²; ¹Shimadzu (China) Co., Ltd., Shanghai, China; ²Tongde Hospital of Zhejiang Province, Hangzhou, China
- ThP 278 **Mass Spectrometry Imaging Studies of Metabolites in Mice Heart Affected With Chagas Disease;** Dan Chen; University of Oklahoma, department of chemistry and biochemistry, Norman, OK
- ThP 279 **On-tissue visualization and quantification of steroid hormones using MALDI-2 in animal models of benign prostatic hyperplasia;** Hannah N. Miles^{1,2,3}; Ana Lucila Bautista-Ruiz^{2,3}; Teresa T. Liu^{2,3}; William A. Ricke^{2,3,4}; Lingjun Li^{4,5}; ¹UW-Madison School of Pharmacy, Madison, WI; ²Department of Urology, University of Wisconsin-Madison, Madison, WI; ³George M. O'Brien Center, University of Wisconsin-Madison, Madison, WI; ⁴School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ⁵Department of Chemistry, University of Wisconsin - Madison, Madison, WI
- ThP 280 **Distribution of active pharmaceutical ingredients in *Forthysia Suspensa* and quality control with mass spectrometry imaging;** Zhenhe Chen¹; Kaoru Nakagawa²; Jian Su³; Keisuke Shima¹; Yongli Liu³; Rong Lei³; Jing Dong¹; Hao Yuan³; Xiaolei Wang³; Satoshi Kasamatsu⁴; Lei Cao¹; Xiaodong Li¹; ¹Shimadzu China Innovation Center, Beijing, China; ²Healthcare Solution Unit, Solutions Center of Excellence, Shimadzu Corporation, Kyoto, Japan; ³Hebei Institute for Drug and Medical Device Control, Shijiazhuang, China; ⁴MS Business Unit, Life Science Business Department, Shimadzu Corporation, Kyoto, Japan
- ThP 281 **On-tissue Derivatization for Mass Spectrometry Imaging of Fatty Acids with Enhanced Detection Sensitivity in Alzheimer's Disease Brain;** Malik Ebbini¹; Hua Zhang¹; Peng-Hsuan Huang²; Lingjun Li^{1,2}; ¹School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ²Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- ThP 282 **Mapping the distribution of sterols in the mouse brain - integrating mass spectrometry imaging with the Allen Mouse Brain Atlas;** Nico Verbeeck¹; Maria José Q Mantas¹; Eylan Yutuc²; Alice Ly¹; William J Griffiths²; Marc Claesen¹; Yuqin Wang²; ¹Aspect Analytics, Genk, Belgium; ²Swansea University Medical School, Swansea, United Kingdom
- ThP 283 **In Situ Free Radical Epoxidation with Laser Desorption Ionization for Mass Spectrometry Imaging of Fatty Acid Isomers;** Huimin Ye¹; Ruijun Jian²; Wenpeng Zhang¹; Yu Xia²; Ouyang Zheng¹; ¹Tsinghua University, Beijing, China; ²Tsinghua University, Beijing, China
- ThP 284 **Whole-body imaging of drugs and metabolites in mice by Desorption Electrospray Ionization Mass Spectrometry Imaging;** Christian Janfelt; University of Copenhagen, Copenhagen, Denmark
- ThP 285 **High spatial resolution TIMS MALDI-2 imaging of Dhcr7-KO mice reveal changes in cholesterol biosynthesis;** Ethan Yang¹; Azad Eshghi¹; Amy Li²; Libin Xu²; Shannon Cornett¹; ¹Bruker Daltonics, Billerica, MA; ²University of Washington, Seattle, WA
- ThP 286 **MALDI Mass Spectrometry Imaging of 13C6-Glucose Uptake Measured in TCA Metabolites from Glioblastoma Mouse Brain;** Joshua L Fischer¹; Kari Wilder-Romans²; Ethan Yang¹; Savannah R Snyder¹; Katherine Stumpo¹; Angelica Lin²; Zitong Zhao²; Jie Xu²; Daniel R. Wahl²; ¹Bruker Daltonics, Billerica, MA; ²University of Michigan Ann-Arbor, Ann Arbor, MI
- ThP 287 **Investigating the effect of a COX inhibitor on early pregnancy in a mouse model using imaging mass spectrometry;** Stefania Gitta¹; Eva Szabo¹; Laszlo Mark¹; ¹Institute of Biochemistry and Medical Chemistry, University of Pecs, Pecs, Hungary
- ThP 288 **Evaluating the Effect of Collagen Degradation on Clostridioides difficile Infection in Murine Cecum via Imaging Mass Spectrometry;** Paul Zerebinski¹; Joshua Soto-Ocaña²; Jonathan T. Specker¹; Joseph P. Zackular^{2,3}; Boone M. Prentice¹; ¹University of Florida, Chemistry Department, Analytical Chemistry Division, Gainesville, FL; ²Division of Protective Immunity, Children's Hospital of Philadelphia, Philadelphia, Pennsylvania; ³Department of Pathology and Laboratory Medicine, Perelman School of Medicine, University of Pennsylvania, Philadelphia, Pennsylvania
- ThP 289 **In-Vitro Diagnostic Imaging of HepaRG Spheroids by DESI-Tandem Quadrupole MS;** Mark Towers¹; Lisa Reid¹; Joanne Ballantyne¹; Alicia Rosell-Hidaglo²; Kirsten Headspith²; ¹Waters Corporation, Wilmslow, United Kingdom; ²Cyprotex Ltd., Alderley Park, United Kingdom
- ThP 290 **Spatiotemporal study of lipid biosynthesis in the mutant seeds of *Arabidopsis thaliana* via 13C labeling and MALDI-MSI;** Anna M Uhlmansiek¹; Andrew E Paulson¹; Young-Jin Lee¹; ¹Iowa State University, Ames, IA
- ThP 291 **A new multimodal desorption electrospray ionisation workflow enabling visualisation of lipids and biologically relevant elements in a single tissue section;** Melanie Bailey¹; Catia D S Costa¹; Janella M De Jesus²; Josephine Bunch²; ¹University of Surrey, Guildford, United Kingdom; ²National Physical Laboratory, Teddington, United Kingdom
- ThP 292 **Mass spectrometry imaging of immune response in human papillomavirus-associated versus carcinogen-driven head and neck squamous cell carcinoma;** William Temple Andrews¹; Aleksandra Ogurtsova²; Mike Mikula²; Ogechi Nwankwoala²; Liz Engle²; Carole Fakhry²; R. Alex Harbison²; Maureen Kane¹; ¹University of Maryland School of Pharmacy, Baltimore, MD; ²Johns Hopkins Hospital, Baltimore, MD
- ThP 293 **Exploring a Human-Relevant Mouse Model for Detecting and Quantifying Medical Therapeutics for Organophosphate Toxicity in the Brain using MALDI-MSI;** Samantha Carriero^{1,2}; Benjamin Wadsworth²; C. Linn Cadieux²; Caitlin M. Tressler³; ¹Oak Ridge Institute of Science Education, Oak Ridge, TN; ²U.S. Army Medical Research Institute of Chemical Defense, Gunpowder, Maryland; ³Johns Hopkins University School of Medicine, Baltimore, MD
- ThP 294 **Assessing methods and performance for glycan imaging of human tissues;** David T. Reeves^{1,2}; Martin Dufresne^{1,3}; Madeline E. Colley^{1,3}; Lukasz G. Migas⁴; Audra M. Judd^{1,3}; Jamie L. Allen^{1,3}; Raf Van De Plas⁴; Jeffrey M. Spraggins^{1,2,3}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands

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- ThP 295 **Multilevel human secondary lymphoid immune system compartmentalization revealed by complementary multiplexing and mass spectrometry imaging;** Benjamin L. Oylar¹; Jefferson Valencia-Davila²; Eirini Moysi²; Adam Molyvdas²; Kalliopi Ioannidou³; Kylie March²; David Ambrozak²; Laurence De Leval³; Giulia Fabozzi²; Amina Woods²; Richard Koup²; Constantinos Petrovas³; ¹*NIH, Gaithersburg, MD*; ²*National Institute of Allergy and Infectious Diseases, Bethesda, MD*; ³*Lausanne University Hospital, Lausanne, Switzerland*
- ThP 296 **Mapping distribution of an alkylamine in tissue for restoration of an Immune-permissive microenvironment;** Danielle Stolley¹; Natalie Fowlkes¹; Maria Sophia Stenkamp¹; Erin H Seeley²; Erik Cressman¹; ¹*MD Anderson Cancer Center, Houston, TX*; ²*University of Texas at Austin, Austin, TX*
- ThP 297 **High Resolution Molecular Mapping of Alzheimer's disease and Cerebral Amyloid Angiopathy (CAA) with MALDI IMS and IHC;** Cody R Marshall^{1,2,3}; Claire F Scott^{2,3,4}; Lissa Ventura-Antunes^{5,6}; Wilber Romero-Fernandez^{5,6}; Alena Shostak^{5,6}; Lukasz G Migas^{2,7}; Martin Dufresne^{2,3,8}; Nathan H Patterson^{2,3,8}; Raf Van De Plas^{2,3,7}; Matthew S Schrag^{5,6}; Jeffrey M Spraggins^{1,2,3,4,8,9}; ¹*Chemical Physical Biology Program, Vanderbilt University School of Medicine, Nashville, TN*; ²*Biomolecular Multimodal Imaging Center, Vanderbilt University, Nashville, TN*; ³*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*; ⁴*Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN*; ⁵*Department of Neurology, Vanderbilt University, Nashville, TN*; ⁶*Cerebral Amyloid Angiopathy Clinic, Vanderbilt University Medical Center, Nashville, TN*; 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*
- ThP 298 **Multi-Reflecting Time-of-Flight Mass Spectrometry Imaging of an Osteosarcoma Tumour Model to Inform Drug Development;** Sophie M. Pearce¹; Neil A. Cross²; Laura M. Cole²; David P. Smith²; James I. Langridge³; Emmanuelle Claude³; Lucy E. Flint⁴; Richard Goodwin⁴; Malcolm R. Clench²; ¹*Sheffield Hallam University, Sheffield, United Kingdom*; ²*Sheffield Hallam University, Sheffield, United Kingdom*; ³*Waters Corporation, Wilmslow, United Kingdom*; ⁴*AstraZeneca, Cambridge, United Kingdom*
- ThP 299 **MALDI-2 MSI of temozolomide distribution and metabolic dysregulation within a murine patient-derived xenograft model of glioblastoma;** Krishna P.L. Bhat¹; Nancy Milam¹; Silvana Valdenbenito^{2,3}; Eliseo Eugenin^{2,3}; Brendan Prideaux^{2,3}; ¹*MD Anderson Cancer Center, Division of Pathology Lab-Medicine, Department of Pathology, Houston, Texas*; ²*University of Texas Medical Branch at Galveston, Galveston, TX*; ³*Department of Neurobiology, Galveston, TX*
- ThP 300 **TOPICAL DELIVERY OF ANTIFUNGAL DRUGS WITH NANO-VESICULAR FORMULATIONS CHARACTERIZED BY DESI-MSI;** Ravit Yakobi¹; Elka Toutou¹; Hiba Natshah¹; Katy Marquis¹; ¹*The Hebrew University of Jerusalem, Jerusalem, Israel*
- ThP 301 **Localization of Molecular Changes Due to Ionizing Radiation Exposure in a Model Teleost by Mass Spectrometry Imaging;** Yixuan Wu¹; Franklin E. Leach III¹; ¹*University of Georgia, Athens, GA*
- ThP 302 **Spatiotemporal Phenotypic Analysis of a Teinturier Grape Cultivar with Atmospheric Pressure Matrix-assisted Laser Desorption Ionization (AP-MALDI) Mass Spectrometry Imaging;** Vishal Mahale^{1,2}; Sujata Chatterjee³; Nasiruddin Shaikh³; Madhuri Gupta^{1,2}; Konstantin Novoselov¹; Eugene Moskovets¹; Kaushik Banerjee³; Nivedita Bhattacharya^{1,2}; Venkateswarlu Panchagnula¹; ¹*MassTech, Inc., Columbia, MD*; ²*Barefeet Analytics Private Limited, Pune, India*; ³*ICAR-National Research Centre for Grapes, Pune, India*
- ThP 303 **Enhanced molecular coverage, resolution and speed for in-situ pharmaceutical tablet MSI analysis by combining DESI and MALDI using multi-reflecting Q-ToF.;** Emmanuelle Claude¹; Wei Rao¹; Laurent Bultel²; Noelle Elliott³; Tristan Renaud²; Joanne B Ballantyne¹; ¹*Waters Corporation, Wilmslow, United Kingdom*; ²*Technologie Servier, Orleans, France*; ³*Waters corp, milford, MA*
- ThP 304 **Spatial proteomics at subcellular resolution enabled by integration of deep UV ablation with nanoPOTS sample preparation;** Piliang Xiang¹; Andrey Liyu¹; Yumi Kwon¹; Dehong Hu¹; William Chrisler¹; Sarah Williams¹; Dušan Veličković¹; Lye Meng Markillie¹; Ljiljana Paša-Tolić¹; Ying Zhu²; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*Genentech Inc, South San Francisco, CA*
- ThP 305 **Three-dimensional proteome mapping of human pancreatic islet microenvironment defines cell type localizations at 50-µm resolution;** Yumi Kwon¹; Sarah M Williams¹; Jing Chen²; Jeremy C Clair¹; Dehong Hu¹; Lye Meng Markillie¹; Andrey V Liyu¹; Karl K Weitz¹; Ronald J Moore¹; Ernesto S Nakayasu¹; Martha Campbell-Thompson²; Clayton Mathews²; Ying Zhu^{1,3}; Wei-Jun Qian¹; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*University of Florida, Gainesville, FL*; ³*Genentech Inc., South San Francisco, CA*
- ThP 306 **Identifying modules of co-regulated metabolites through large-scale analyses of public spatial metabolomics data in METASPACE;** Tim D Rose¹; Kevin Titeca¹; Sergii Mamedov¹; Lucas Maciel Vieira¹; Sergio Triana^{1,2,3,4,5}; Theodore Alexandrov^{1,6,7,8}; ¹*Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany*; ²*Broad Institute of MIT and Harvard, Cambridge, MA*; ³*Institute for Medical Engineering and Science, MIT, Cambridge, MA*; ⁴*Department of Chemistry, MIT, Cambridge, MA*; ⁵*Ragon Institute of MGH, MIT and Harvard, Cambridge, MA*; ⁶*Metabolomics Core Facility, Heidelberg, Germany*; ⁷*Molecular Medicine Partnership Unit, Heidelberg, Germany*; ⁸*Bio Studio, BiInnovation Institute, Copenhagen, Denmark*
- ThP 307 **Tumor heterogeneity of glioblastoma analyzed via SpatialOMx and HiPLEX-IHC MALDI Imaging;** Corinna Henkel¹; Signe Frost Frederiksen¹; Katherine A. Stumpo²; Matthias Szesny¹; Jörg W. Bartsch³; Melanie C. Föll^{4,5}; Oliver Schilling^{4,5}; ¹*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*; ²*Bruker Daltonics, Billerica, MA*; ³*Department of Neurosurgery, University of Marburg, Marburg, Germany*; ⁴*Institute for Surgical Pathology, Medical Center, University of Freiburg, Freiburg, Germany*; ⁵*Faculty of Medicine, University of Freiburg, Freiburg, Germany*
- ThP 308 **Tetramodal Chemical Imaging Delineates the Lipid-Amyloid Peptide Interplay at Single Plaques in Transgenic Alzheimer's Disease Models;** Junyue Ge¹; Srinivas Koutarapu¹; Durga Jha¹; Henrik Zetterberg^{1,2,3,4,5,6}; 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*UK Dementia Research Institute at University College London, London, United Kingdom*; ⁵*Hong Kong Center for Neurodegenerative Diseases, Hong Kong, China*; ⁶*University of Wisconsin, Madison, WI*
- ThP 309 **Optimized Combination of MALDI MSI and Immunofluorescence;** Catelynn C Ridge¹; Elizabeth K. Neumann¹; ¹*UC Davis, Davis, CA*
- ThP 310 **Large-Scale Interlaboratory Comparison of Imaging Mass Spectrometry Protocols for Spatial Untargeted Metabolomics;** Veronika Saharuka¹; Måns Ekelöf¹; Lachlan Stuart¹; Lucas M. Vieira¹; Martijn R Molenaar¹; Alberto Bailoni¹; Katja Ovchinnikova²; Tobias Bausbacher³; Dennis Jakob⁴; Mary King⁵; Max Müller⁶; Crystal Pace⁷; Fernanda E. Pinto⁸; Nicole Strittmatter⁹; Jens Soltwisch¹⁰; Dušan Veličković¹¹; Janina Oetjen¹²; Christopher Anderton¹¹; Livia

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- S. Eberlin¹³; Richard Goodwin⁹; Christian Janfelt⁸; Manuel Liebeke⁴; David C. Muddiman⁷; Bernhard Spengler⁶; Klaus Dreisewerd¹⁰; Carsten Hopf^{3, 14, 15}; Theodore Alexandrov^{1, 16, 17, 18}; ¹Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany; ²Department for BioMedical Research, University of Bern, Bern, Switzerland; ³CeMOS - Center for Mass Spectrometry and Optical Spectroscopy, Mannheim, Germany; ⁴Max Planck Institute for Marine Microbiology, Bremen, Germany; ⁵University of Texas at Austin, Austin, TX; ⁶Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Gießen, Germany; ⁷Department of Chemistry, North Carolina State University, Raleigh, NC; ⁸Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; ⁹AstraZeneca, Cambridge, United Kingdom; ¹⁰Institute of Hygiene, University of Münster, Münster, Germany; ¹¹Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; ¹²Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ¹³Department of Surgery, Baylor College of Medicine, Houston, TX; ¹⁴Medical Faculty of Heidelberg University, Heidelberg, Germany; ¹⁵Mannheim Center for Translational Neuroscience (MCTN), Medical Faculty Mannheim, Heidelberg University, Mannheim, Germany; ¹⁶Metabolomics Core Facility, Heidelberg, Germany; ¹⁷Molecular Medicine Partnership Unit, Heidelberg, Germany; ¹⁸Bio Studio, BioInnovation Institute, Copenhagen, Denmark
- ThP 311 **Nano-DESI mass spectrometry imaging of intact protein-metal complexes associated with the pathogenesis of amyotrophic lateral sclerosis**; Oliver J. Hale¹; Tyler R. Wells²; Richard J. Mead²; Helen J. Cooper¹; ¹University of Birmingham, Birmingham, United Kingdom; ²Sheffield Institute for Translational Neuroscience, University of Sheffield, Sheffield, United Kingdom
- ThP 312 **Coupling Immunohistochemistry with MALDI-MS Imaging: A Multidimensional Imaging Strategy for Mapping Molecular Signatures in the Alzheimer's Disease Brain**; Kelly H. Lu¹; Hua Zhang²; Gargey B. Yagnik³; Mark J. Lim³; Kenneth J. Rothschild³; Andrew J. Schneider^{4, 5}; Luigi Puglielli^{4, 5}; Lingjun Li^{1, 2}; ¹University of Wisconsin-Madison, Department of Chemistry, Madison, WI; ²University of Wisconsin-Madison School of Pharmacy - Madison, WI, Madison, WI; ³AmberGen, Inc., Billerica, MA; ⁴University of Wisconsin-Madison, Department of Medicine, Madison, WI; ⁵Waisman Center, University of Wisconsin-Madison, Madison, WI
- ThP 313 **Ultrahigh Mass Resolving Power Mass Spectrometry Imaging Approaches to Address Molecular and Topographic Complexity**; Gregory W Vandergriff¹; Kevin J Zemaitis¹; Arunima Bhattacharjee¹; Dušan Veličković¹; Jessica K Lukowski¹; Ljiljana Paša-Tolić¹; William Kew¹; Christopher Anderton¹; ¹Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington
- ThP 314 **Novel Myc-driven metabolic vulnerability identified by multimodal mass spectrometry imaging**; Peter Kreuzaler¹; Paolo Inglese²; Avinash Ghanate¹; Erska Gjelađi¹; Vincen Wu³; Yulia Panina¹; Andres Mendez-Lucas¹; Catherine MacLachlan¹; Neill Patani¹; Catherine B Hubert¹; Helen Huang³; Gina Greenidge⁴; Oscar M Rueda⁵; Adam J Taylor⁴; Evdokia Karali⁶; Emine Kazanc³; Amy Spicer¹; Wei Lin¹; Daria Thompson¹; Mariana Silva Dos Santos¹; Enrica Calvani¹; Nathalie Legrave¹; James K Ellis¹; Rory T Steven⁷; Wendy Greenwood⁵; Mary Green¹; Emma Nye¹; Emma Still¹; Simon T Barry⁸; Richard J A Goodwin⁸; Alejandra Bruna⁶; Carlos Caldas⁵; James Macrae¹; Luiz Pedro Sorio de Carvalho¹; George Pouligiannis⁶; Greg McMahon⁴; Zoltan Takats³; Josephine Bunch⁴; Mariia Yuneva¹; ¹The Francis Crick Institute, London, United Kingdom; ²Imperial College London, London, United Kingdom; ³Imperial College London, London, United Kingdom; ⁴National Physical Laboratory, Teddington, United Kingdom; ⁵University of Cambridge, Cambridge, United Kingdom; ⁶The Institute of Cancer Research, London, United Kingdom; ⁷National Physical Laboratory, London, United Kingdom; ⁸AstraZeneca, Cambridge, United Kingdom
- ThP 315 **Mobility-Modulated Sequential Dissociation of Multiple Precursors (SDIMP) for Highly Multiplexed MS/MS Imaging**; Yao Qian¹; Xiaoxiao Ma¹; Zheng Ouyang¹; ¹Department of Precision Instrument, Tsinghua University, Beijing, China
- ThP 316 **Direct detection of lipid changes on cultured cells using imaging secondary ion mass spectrometry following chemical and/or biological perturbation**; John Fletcher; ¹University of Gothenburg, Gothenburg, Sweden
- ThP 317 **Advancing the Construction of High Spatial Resolution 3-D Multimodal Molecular Atlases with the Aid of Data-Driven Image Fusion**; Olof Gerdur Isberg^{1, 2}; Melissa A Farrow^{1, 3, 4}; Lukasz G Migas⁵; Madeline Colley^{1, 3}; Jamie L. Allen^{1, 3}; Haichun Yang^{4, 6}; Mark P De Caestecker^{2, 7}; Raf Van De Plas^{1, 3, 5}; Jeffrey M Spraggins^{1, 2, 3}; ¹Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; ²Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; ³Department of Biochemistry, Vanderbilt University, Nashville, TN; ⁴Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; ⁵Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ⁶Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; ⁷Department of Medicine, Vanderbilt University, Nashville, TN
- ThP 318 **Scalable multimodal workflow for spatial glycan analysis of archival formalin-fixed paraffin-embedded (FFPE) human tissue using MALDI, MIBI-TOF, and spatial transcriptomics**; Ke Xuan Leow¹; Xiaowei Lu¹; Marc Bosse¹; Richard R Drake²; Peggy M. Angel²; Sean Bendall¹; Mike Angelo¹; ¹Stanford University, Stanford, CA; ²Medical University of South Carolina, Charleston, SC
- ThP 319 **Exploring MALDI-MSI with Higher Metabolite Coverage and Its Application in Spatial Metabolomics**; Jia Yi¹; Joe L. Rowles¹; Leah P. Shriver¹; Gary J. Patti¹; ¹Washington University in St. Louis, St. Louis, MO
- ThP 320 **Micro-scaffold Assisted Spatial Proteomics (MASP) with Substantially Improved Spatial Resolution and Throughput for Whole Tissue Mapping**; Shihan Huo¹; Min Ma²; Shuo Qian²; Ming Zhang¹; Jie Pu¹; Xiaoyu Zhu¹; Sailee Rasam¹; Jun Qu¹; ¹University at Buffalo, Buffalo, NY; ²Roswell Park Comprehensive Cancer Institute, Buffalo, NY
- ThP 321 **Aberrant Lipid Metabolism in the Orthotopic Mouse Glioma: A MALDI-MS Imaging and Lipidomic Study**; Hai-Yan J Wang¹; Chiung-Yin Huang^{2, 3}; Kuo-Chen Wei^{2, 3, 4, 5}; Kuo-Chen Hung⁶; ¹National Sun Yat-Sen University, Kaohsiung City, Taiwan; ²Neuroscience Research Center, Chang Gung Memorial Hospital, Taoyuan, Taiwan; ³Department of Neurosurgery, New Taipei Municipal TuCheng Hospital, New Taipei City, Taiwan; ⁴Department of Neurosurgery, Chang Gung Memorial Hospital, Taoyuan, Taiwan; ⁵School of Medicine, Chang Gung University, Taoyuan, Taiwan; ⁶Department of Surgery, Kaohsiung Chang Gung Memorial Hospital, Kaohsiung, Chang Gung University College of Medicine, Kaohsiung, Taiwan
- ThP 322 **Dissecting Immunometabolism of Dilated Cardiomyopathy (DCM) on delta-sarcoglycan deficient hamster model with thoracic Imaging Mass Spectrometry (tIMS)**; Maiko Okamura¹; Shinichi Yamaguchi²; Takushi Yamamoto²; Ryo Inoue³; Laura Yuriko González – Teshima⁴; Keisuke Hakamada⁴; Kisaki Amemiya⁵; Kenji Minatoya⁴; Hidetoshi Masumoto⁴; Satoru Noguchi⁶; Ichizo Nishino⁶; Hatsue Ueda^{5, 7}; Masaya Ikegawa¹; ¹Department of Life and Medical Systems, Doshisha University, Kyotanabe-city, Japan; ²Shimadzu Corporation, Kyoto-city, Japan; ³Faculty of Agriculture, Setsunan University, Hirakata-city, Japan; ⁴Department of

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- Cardiovascular Surgery, Graduate School of Medicine, Kyoto University, Kyoto-city, Japan; ⁵Department of Pathology, National Cerebral and Cardiovascular Center, Suita-city, Japan; ⁶Department of Neuromuscular Research, National Center of Neurology and Psychiatry, Kodaira-city, Japan; ⁷Department of Diagnostic Pathology, Hokusetsu General Hospital, Takatsuki-city, Japan
- ThP 323 **Optimization and Application of Single Cell Lipidomics Using Nanocapillary Sampling and Ultra High Performance Liquid Chromatography Mass Spectrometry**; Kyle Saunders¹; Holly-May Lewis¹; Catia Costa^{1,2}; Johanna Von-Gerichten¹; Priyanka Gupta³; Eirini Velliou³; Melanie Bailey¹; ¹University of Surrey, Guildford, United Kingdom; ²Surrey Ion Beam Centre, Guildford, United Kingdom; ³University College London, London, United Kingdom
- ThP 324 **Metabolomes reveal EGT and IPA as intervenable biomarkers for cancer-therapeutics-related cardiac dysfunction (CTRCD) in breast cancer patients and mouse models**; Lik Hang Wu¹; Muthu K. Shanmugam¹; Pakkiri Leroy Sivappiragasam¹; H. Ling Lieng¹; Hyungwon Choi¹; Eugene Goh¹; Li Ling Tan²; Yoon Sim Yap³; Soo Chin Lee⁴; A. Mark Richards¹; Chester L. Drum¹; ¹National University of Singapore, Singapore, Singapore; ²National University Heart Centre, Singapore, Singapore; ³Department of Medical Oncology at National Cancer Centre Singapore, Singapore, Singapore; ⁴National University Cancer Institute, Singapore, Singapore
- ThP 325 **GraphCCS: Prediction of Collision Cross-Section for Metabolites Using Graph Neural Network**; Hsin-Hsiang Chung¹; Cheng-Chih Hsu¹; ¹Department of Chemistry, National Taiwan University, Taipei City, Taiwan
- ThP 326 **Automated and interpretable machine learning for MS metabolomics: predicting cancer diagnosis**; Olatomiwa O Bifarin¹; Facundo M Fernandez¹; ¹Georgia Institute of Technology, Atlanta, GA
- ThP 327 **All-in-one Data-Processing and Interactive Visualizations of Lipid LC-HRMS/MS Data using LipidMatch 4.0**; Jeremy Koelmel¹; Paul Stelben¹; Bernard Brooks^{2,3}; Jung Suh⁴; Mark Sartain⁵; Timothy J. Garrett⁶; John A. Bowden⁶; Emma E Rennie⁵; Krystal J Godri Pollitt¹; ¹Yale University, New Haven, CT; ²Innovative Omics, Sarasota, FL; ³Mudai Studios, Sarasota, FL; ⁴Denali Therapeutics, San Francisco, CA; ⁵Agilent Technologies, Santa Clara, CA; ⁶University of Florida, Gainesville, FL
- ThP 328 **Untargeted exometabolomics of a fast-growing cyanobacterium Synechococcus elongatus PCC11801 strain in different growth media**; Virmal S. Jain¹; Meghna Srivastava¹; Prajval Nakrani²; Pramod P. Wangikar^{1,2}; ¹Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai, India; ²Clarity Bio Systems India Pvt Ltd, Pune, India
- ThP 329 **Plasma metabolomic profiling reveals metabolites robustly associated with COVID-19 severity and metabolism alterations before, during, and after disease**; Haley Chatelaine¹; Yulu Chen²; John Braisted¹; Su Chu²; Meryl Stav²; Sofina Begum²; Joann Diray-Arce²; Jaleal Sanjak¹; Mengna Huang²; Jessica Lasky-Su²; Ewy Mathe¹; ¹Division of Preclinical Innovation, National Center for Advancing Translational Sciences, National Institutes of Health, Rockville, MD; ²Channing Laboratory, Brigham and Women's Hospital, Harvard Medical School, Boston, MA
- ThP 330 **Development of powerful metabolomics platform for combined of target and non-target analysis**; Hideaki Kasahara¹; Yasuto Yokoi¹; Tadahiro Hoshino¹; Akio Hayashi²; Hitoshi Shimano²; ¹Mitsui Knowledge Industry co., Ltd., Tokyo, Japan; ²Department of Endocrinology and Metabolism, Faculty of Medicine, University of Tsukuba, Tsukuba, Japan
- ThP 331 **DeNox: a visualization tool for LC-MS/MS metabolomics quantitation data**; Jie-Wei Chiu¹; Sin-Chen Chiang¹; Hui-Yin Chang²; ¹Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan; ²Department of Biomedical Sciences and Engineering, Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan
- ThP 332 **End to End Interpretable Deep Learning Workflow for Untargeted Metabolomics**; Miao Yu¹; Rohit Tripathy¹; Brian Hoffmann²; Yi Li¹; Vivek Philip¹; ¹The Jackson Laboratory, Farmington, CT; ²The Jackson Laboratory, Bar Harbor, ME
- ThP 333 **A workflow to track and normalize the abundance of unknown and known metabolites across LC/MS methods**; Ethan Stancliffe¹; Michaela Schwaiger-Haber¹; Gary J. Patti¹; ¹Washington University in Saint Louis, Saint Louis, MO
- ThP 334 **Skyline Processing Workflow for Lipidomics Using High Resolution Ion Mobility Mass Spectral Data with Mobility Aligned Fragmentation**; Lauren C Rover¹; Rachel Harris¹; Daniel DeBord¹; ¹MOBILion Systems, Inc, Chadds Ford, PA
- ThP 335 **A deep lipidomics strategy for evaluation of cancer therapy**; Haoyue Zhang¹; Yikun Liu¹; Donghui Zhang¹; Wenpeng Zhang¹; Zheng Ouyang¹; ¹Tsinghua University, Beijing, China
- ThP 336 **Enzymatic Dysregulation Estimation using Lipid Network Analysis**; Tim D Rose^{1,2}; Nikolai Köhler¹; Lisa Falk¹; Lucie Klischat¹; Olga E Lazareva^{2,3}; Josch K Pauling¹; ¹LipiTUM, Technical University of Munich, Freising, Germany; ²EMBL, Heidelberg, Germany; ³German Cancer Research Center (DKFZ), Heidelberg, Germany
- ThP 337 **PAMDA: Publicly Available Metabolomics Dataset Alignment and Analysis of Human Urine Measured by RPLC-MS**; Hani Habra¹; Yamil Simon¹; Tytus D. Mak¹; ¹NIST, Gaithersburg, MD
- ThP 338 **Fragmentation Site Prediction for Non-Targeted Metabolomics using Graph Neural Networks**; Yannek Nowatzky¹; Philipp Benner¹; Thilo Muth¹; ¹Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany
- ThP 339 **MS/MS-centric data processing with SIRIUS 6**; Kai Dührkop¹; Markus Fleischauer¹; Marcus Ludwig¹; Martin Andre Hoffmann¹; Fleming Kretschmer¹; Sebastian Böcker¹; ¹Friedrich-Schiller-University Jena, Jena, Germany
- ThP 340 **Lipid-class specific internal standard normalization of HILIC-MS/MS data embedded into untargeted data processing and interactive exploration**; Edward Rudt¹; Viola Jeck²; Konstantin Schwarze²; Ansgar Korf²; Matthew R. Lewis²; Heiko Hayen¹; Nikolas Kessler²; ¹Institute of Inorganic and Analytical Chemistry, Münster, Germany; ²Brüker Daltonics GmbH & Co. KG, Bremen, Germany
- ThP 341 **Interactive Design and Application of MassQL Queries after Preprocessing for the Annotation of PFAS in LC-TIMS-PASEF data**; Andrea Kiehne¹; Silke Bodendiek¹; Sofie Weinkouff¹; Mingxun Wang²; Heiko Neuweger¹; Nikolas Kessler¹; ¹Brüker Daltonics GmbH & Co. KG, Bremen, Germany; ²Department of Computer Science and Engineering, University of California Riverside, Riverside, CA
- ThP 342 **LipidDetective: a Deep Learning Framework for the Detection of Lipid Species in Mass Spectra**; Vivian J Wuertl¹; Nikolai Köhler¹; Florian Molnar¹; Michael Witting^{1,2}; Josch K Pauling¹; ¹Technical University of Munich, Freising, Germany; ²Helmholtz Zentrum München – German Research Center for Environmental Health, Neuherberg, Germany
- ThP 343 **The Evolving Open Access Metabolomics Resource MetaboLights**; Claire C O'Donovan¹; Callum Martin¹; Ozgur Yurekten¹; Felix Amaladoss¹; Mark Williams¹; Thomas Payne¹; ¹EMBL-EBI, Hinxton, United Kingdom
- ThP 344 **Incorporation of metabolite identification confidence into pathway analysis when processing untargeted metabolomics data improves enriched pathway discovery**; Blake E. Sells¹; Ethan Stancliffe¹; Jacob S. Bedia¹; Michaela Schwaiger-Haber¹; Leah P. Shriver¹; Gary J. Patti¹; ¹Washington University in St. Louis, St. Louis, MO

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- ThP 345 **High-fidelity and high-performance LC-MS metabolomics data processing using asari**; [Shuzhao Li](#)^{1,2}; Amnah Siddiqua¹; Maheshwor Thapa¹; Shujian Zheng¹; ¹Jackson Laboratory, Farmington, CT; ²University of Connecticut School of Medicine, Farmington, CT
- ThP 346 **MSPaint: A versatile Python package for visualizing mass spectrometry data**; [Shaurya Chanana](#)¹; John T. Prince¹; ¹Enveda Biosciences, Boulder, CO
- ThP 347 **Combining MS2 and MS3 fragmentation spectra for the annotation of complex sphingolipids**; [Brandon Y. Lieng](#)¹; Jeremy K. Chan¹; Nicholas S. Ly¹; Hannes L. Röst¹; J. Rafael Montenegro-Burke¹; ¹Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON
- ThP 348 **Glycoprotein analysis benefits from direct feature extraction and compound identification via correlation of experimental and accurately simulated Orbitrap mass spectra**; [Konstantin Nagornov](#)¹; Anton N. Kozhinov¹; Sergey Vakhrushev²; Yury O. Tsybin¹; ¹Spectroswiss, Lausanne, Switzerland; ²University of Copenhagen, Copenhagen, Denmark
- ThP 349 **Reproducibility and challenges in analysis of large urine metabolomics datasets**; [Stephen Barnes](#)¹; Landon S. Wilson¹; Taylor F. Berryhill¹; Shaoyong Su²; ¹University of Alabama at Birmingham, Birmingham, AL; ²Augusta university, Augusta, Georgia
- ThP 350 **SpectraSpectre: An implementation of MassQL for rapid querying of MS data**; [Dylan J Johnson](#)¹; Alan K Jarmusch²; ¹Integrative Bioinformatics Support Group, National Institute of Environmental Health Sciences, National Institutes of Health, Durham, North Carolina; ²Metabolomics Core Facility, Immunity, Inflammation, and Disease Laboratory, Division of Intramural Research, National Institute of Environmental Health Sciences, National Institutes of Health, Durham, North Carolina
- ThP 351 **Library-scale assessment of spectral quality of MS/MS spectra**; Christoph A. Kretzler¹; J Taylor¹; Tobias Kind¹; Pelle Simpson¹; [Sarah E Haynes](#)¹; David Healey¹; ¹Enveda Biosciences, Boulder, CO
- ThP 352 **Ground-truth evaluation of high dimensional feature calling methods**; J Taylor¹; Alex A. Kislukhin¹; Daniel Treen¹; Tobias Kind¹; Sarah Haynes¹; David Healey¹; [John T. Prince](#)¹; ¹Enveda Biosciences, Boulder, CO
- ThP 353 **High-dimensional feature/adduct linking with a noise-tolerant, sparse cosine similarity measure**; [Daniel G.C. Treen](#)¹; John T. Prince¹; ¹Enveda Biosciences, Boulder, CO
- ThP 354 **Noise Filtering in Non-targeted Metabolomics**; [Iqbal Mahmud](#)¹; Anika Patel^{1,2}; Lin Tan¹; Sara A Martinez¹; Bao Tran¹; Bo Wei¹; Rehan Akbani¹; Bradley Broom¹; John Weinstein¹; Philip L Lorenzi¹; ¹MD Anderson Cancer Center, Houston, TX; ²Rice University, Houston, TX
- ThP 355 **MS/MS Spectral Alignment Enables Structural Modification Site Localization**; [Mohammad Reza Zare Shahneh](#)¹; Mingxun Wang²; ¹University of California, Riverside, Riverside, CA; ²University of California Riverside, Riverside, CA
- ThP 356 **Automated Multiple Reaction Monitoring(MRM)-profiling and ozone electrospray ionization (OzESI)-MRM Informatics Platform for High-throughput Lipidomics**; [Connor H Beveridge](#)¹; Sanjay Iyer²; Caitlin E. Randolph¹; Gaurav Chopra¹; ¹Purdue University Department of Chemistry, West Lafayette, IN; ²Purdue University, Dept. of Chemistry, West Lafayette, IN
- ThP 357 **Updates in the MSFragger search engine: facilitating bulk-cell and single-cell proteomics data analysis**; [Fengchao Yu](#)¹; Daniel A. Polasky¹; Andy T. Kong¹; Guo Ci Teo¹; Kevin L. Yang¹; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI
- ThP 358 **Quantification of peptidofoms in data from middle-down proteomics experiments with ProteoformQuant**; [Arthur Grimaud](#)¹; Frederik Haugaard Holck¹; Ole Nørregaard Jensen¹; Veit Stefan Schwämmle¹; ¹University of Southern Denmark, Odense, Denmark
- ThP 359 **Estimating False Discovery Rate During Real-Time Library Search Acquisitions**; [William Barshop](#)¹; Chris McGann²; Devin K Schweppe²; Jesse D. Canterbury¹; ¹Thermo Fisher Scientific, San Jose, California; ²University of Washington, Seattle, WA
- ThP 360 **AutoMod: a new solution for uncovering protein post-translational modifications**; [Hui-Yin Chang](#)¹; Jie-Wei Chiu²; Yi-Fan Chen³; Shuo-fu Chen⁴; Chia-Feng Tsai⁵; ¹Department of Biomedical Sciences and Engineering, Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan; ²Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan; ³Interdisciplinary Program of Engineering, National Central University, Taoyuan, Taiwan; ⁴Department of Oncology, Taipei Veterans General Hospital, Taipei, Taiwan; ⁵Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA
- ThP 361 **A Crustacean Neuropeptide Spectral Library for Application in Data-Independent Acquisition Peptidomic Workflows**; [Lauren Fields](#)¹; Min Ma¹; Kellen Delaney¹; Ashley Phetsanhad¹; Lingjun Li¹; ¹University of Wisconsin-Madison, Madison, WI
- ThP 362 **CONGA: Combining open and narrow searches with group-wise analysis**; Jack Freestone¹; [William Noble](#)²; Uri Keich¹; ¹University of Sydney, Sydney, Australia; ²University of Washington, Seattle, WA
- ThP 363 **An XIC-centric approach for improved identification, quantification, and reproducibility in proteomic data analyses**; [Guanghui Wang](#)¹; Zheng Zhang¹; Yi Liu¹; Meghan C. Burke¹; Sergey L. Sheetlin¹; Stephen E. Stein¹; ¹NIST, Gaithersburg, MD
- ThP 364 **Generating spectral libraries using experimental target spectra and ProSIT predicted decoy spectra**; [Robert W Seymour](#)¹; Andy Lin¹; ¹Pacific Northwest National Laboratory, Richland, WA
- ThP 365 **Information content assessment of peptide fragmentation spectra using deep learning models**; [Zahra Elhamraoui](#)^{1,2}; Eva Borrás²; Mathias Wilhelm³; Eduard Sabidó^{1,2}; ¹Center for Genomic Regulation, Barcelona, Spain; ²Universitat Pompeu Fabra Barcelona, Barcelona, Spain; ³Technical University of Munich, Freising, Germany
- ThP 366 **Improvement of noncanonical peptide identification using local RNA expression value in MHC-I immunopeptidomics**; [Seunghyuk Choi](#)¹; Seunghyun Han¹; Eunok Paek¹; ¹Hanyang University, Seoul, South Korea
- ThP 367 **ProSIT-PTM: One model to predict them all**; [Wassim Gabriel](#)¹; Vitor Sternlicht¹; Omar Shouman¹; Rodeina Mohamed¹; Daniel P. Zolg²; Ludwig Lautenbacher¹; Bernhard Kuster²; Mathias Wilhelm¹; ¹Computational Mass Spectrometry, Technical University of Munich, Freising, Germany; ²Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany
- ThP 368 **High-throughput Automated Muropeptide Analysis (HAMA) Reveals Peptidoglycan Composition of Gut Microbes**; [Ya-Chen Hsu](#)¹; Pin-Rui Su^{1,2}; Lin-Jie Huang¹; Cheng-Chih Hsu¹; ¹Department of Chemistry, National Taiwan University, Taipei, Taiwan; ²Department of Molecular Genetics, Erasmus University Medical Center, Rotterdam, Netherlands
- ThP 369 **SpecGlobX: a fast tool for aligning mass spectra in large proteomics datasets, capturing dissimilarities arising from multiple complex peptides modifications**; Grégoire Prunier^{1,2}; Mehdi Cherkaoui^{1,3}; Albane Lysiak^{1,4}; Olivier Langella⁵; Mélisande Blein-Nicolas⁵; Virginie Lollier^{1,3}; Emile Benoist⁴; Géraldine Jean⁴; [Guillaume Fertin](#)⁴; Hélène Rogniaux^{1,3}; Dominique Tessier^{1,3}; ¹INRAE, PROBE research infrastructure, BIBS facility F-44300, Nantes, France; ²INRAE UR1268 Biopolymères Interactions Assemblage F-44316, Nantes, France; ³INRAE UR1268 Biopolymères Interactions Assemblage F-44316 Nantes, Nantes, France; ⁴LS2N, Nantes Université, Nantes Cedex 3, France; ⁵Université Paris-Saclay, INRAE, CNRS,

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- AgroParisTech, GQE - Le Moulon, PAPPSO, F-91190, Gif-Sur-Yvette, France
- ThP 370 **Precise and accurate real-time de novo sequencing of timsTOF data with the Novor algorithm on the PaSER platform;** Rui Zhang¹; Qixin Liu¹; Mingjie Xie¹; Dennis Trede²; Tharan Srikumar³; Jonathan Krieger³; Bin Ma¹; George Rosenberger⁴; ¹Rapid Novor Inc., Kitchener, ON; ²Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ³Bruker Ltd., Milton, ON; ⁴Bruker Switzerland AG, Faellanden, Switzerland
- ThP 371 **An assessment of the replicability and sample number requirements of differential expression analysis in bottom-up proteomics;** Steven Tavis^{1,2}; Diana Ramirez^{1,2}; Matthew J Keller^{1,2}; Frank Löffler¹; Robert L Hettich^{1,2}; ¹University of Tennessee, Knoxville, TN; ²Oak Ridge National Laboratory, Oak Ridge, TN
- ThP 372 **An integrative proteomics result viewer for FragPipe;** Kai Li¹; Fengchao Yu¹; Daniel Polasky¹; Alexey I. Nesvizhskii¹; ¹University of Michigan, Ann Arbor, MI
- ThP 373 **Multiplexed peptide identification via iterative database search;** Chen Qian¹; Seungjin Na¹; Eunok Paek¹; ¹Hanyang University, Seoul, South Korea
- ThP 374 **MS²Rescore 3.0: A modular and user-friendly platform for AI-assisted rescoring of peptide identifications;** Ralf Gabriels^{1,2}; Arthur Declercq^{1,2}; Robbin Bouwmeester^{1,2}; Sven Degroeve^{1,2}; Lennart Martens^{1,2}; ¹VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; ²Department of Biomolecular Medicine, Ghent University, Ghent, Belgium
- ThP 375 **MS²Rescore and Sage enable open modification immunopeptidomics searching;** Arthur Declercq^{1,2}; Robbin Bouwmeester^{1,2}; Aurélie Hirschler³; Christine Carapito³; Sven Degroeve^{1,2}; Lennart Martens^{1,2}; Ralf Gabriels^{1,2}; ¹VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; ²Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; ³Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO) IPHC UMR 7178, Université de Strasbourg, France
- ThP 376 **Spectroscopie: validating peptide spectrum matches by real time visualization of their neighborhoods with an interactive web interface;** Long Wu¹; Ayman Hoque¹; Henry Lam¹; ¹HKUST, Hong Kong, China
- ThP 377 **De novo sequencing of ranid frogs skin peptides with the Twister algorithm;** Kira Vyatkin^{1,2,3,4}; Irina D. Vasileva⁵; Tatyana Y. Samgina⁶; Albert T Lebedev⁵; ¹SPb Academic University, St Petersburg, Russia; ²Saint Petersburg State University, St Petersburg, Russia; ³Saint Petersburg Electrotechnical University "Leti", St Petersburg, Russia; ⁴National Research Center on Addictions, Branch of V. Serbsky NMRCNP, Moscow, Russia; ⁵Lomonosov Moscow State University, Chemistry department, Moscow, Russian Federation
- ThP 378 **Real-Time de novo sequencing of peptide antigens using PaSER™ for 'Run and Done' 4D-immunopeptidomics;** Kirti Pandey¹; Rui Zhang²; Qixin Liu²; Mingjie Xie²; Dennis Trede³; Tharan Srikumar⁴; Jonathan R Krieger⁴; Bin Ma²; George Rosenberger⁵; Anthony W. Purcell⁶; ¹Monash University, Clayton, Australia; ²Rapid Novor Inc., Kitchener, ON; ³Bruker Dalton's GmbH & Co KG, Bremen, Germany; ⁴Bruker Ltd., Milton, ON; ⁵Bruker Switzerland AG, Fällanden, Switzerland; ⁶Monash University, Clayton, Australia
- ThP 379 **Algorithm Development for Analysis of Human O-GlcNAcylated Protein using LC-MS/MS;** Dasom An¹; Jin Young Kim²; Heeyoun Hwang²; ¹Korea Basic Science Institute, Cheongju-si, South Korea; ²Korea Basic Science Institute, Cheongju, South Korea
- ThP 380 **Investigating the Lipidome of ATP10d Corrected Murine Models Using LC-IM-MS with High Resolution Ion Mobility;** David C. Koomen¹; Jody C. May¹; Alexander J. Mansueto¹; Todd R. Graham¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN
- ThP 381 **Noncovalent Copper Complexation to Differentiate Drug Enantiomers by Conventional and High Resolution Ion Mobility-Mass Spectrometry;** Benjamin K Blakley¹; Emanuel Zlibut¹; Allison R Reardon¹; Jody C. May¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN
- ThP 382 **Characterizing the Molecular Composition of Polysorbates by High Resolution Ion Mobility-Mass Spectrometry (HRIM-HRMS);** Kyle E Lira¹; Allison R Reardon¹; Jody C. May¹; John A. McLean¹; ¹Vanderbilt University, Nashville, TN
- ThP 383 **Pushing the Boundaries of Multidimensional Separations: Coupling 2D Chromatography with High-Resolution Structures for Lossless Ion Manipulations (SLIM) IM-MS;** Ralph Aderorho¹; Diana C. Velosa²; Shon P. Neal²; Christopher D. Chouinard¹; ¹Clemson University, Clemson, SC; ²Florida Tech, Melbourne, FL
- ThP 384 **Brain metastasis of lung adenocarcinoma: gangliosidome investigation by ion mobility tandem mass spectrometry;** Mirela Sarbu¹; David E. Clemmer²; Željka Vukelic³; Alina D. Zamfir⁴; ¹National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania; ²Indiana University Bloomington, Bloomington, IN; ³Department of Chemistry and Biochemistry, Faculty of Medicine, University of Zagreb, Zagreb, Croatia; ⁴National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania
- ThP 385 **LC-TIMS-MS based assay for profiling and quantitation of bile acid in human biofluids;** Aiko Barsch¹; Surendar Tadi²; Xuejun Peng³; Elena Chekmeneva⁴; Katie E. Chappell⁴; Niels Goedecke¹; Matthew R. Lewis¹; ¹Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ²Bruker Daltonics, Billerica, MA; ³Bruker Daltonics, San Jose, CA; ⁴National Phenome Centre & Section of Analytical Chemistry, Division of Systems Medicine, Department of Metabolism, Digestion & Reproduction, Imperial College London, London, United Kingdom
- ThP 386 **Autonomous multi-pass and IMSn acquisitions on the Cyclic IMS platform;** Jakub Ujma¹; Kevin Giles¹; Jose De Corral²; Keith Richardson¹; David Langridge¹; Dale Cooper-shepherd¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters Corporation, Milford, MA
- ThP 387 **Coupling droplet microfluidics to cyclic ion mobility mass spectrometry for separation of isomeric small molecules;** Laura I Penabad¹; Devin M. Makey¹; Robert T. Kennedy¹; Brandon T Ruotolo¹; ¹University of Michigan-Ann Arbor, Ann Arbor, MI
- ThP 388 **Applying Ultraviolet Photodissociation to a Low-Pressure Drift Tube Orbitrap Mass Spectrometer to Enhance the Structural Characterization of Intact Native Proteins;** Jamie P Butalewicz¹; James D Sanders¹; Nathan W. Buzitis²; Brian H. Clowers²; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX; ²Washington State University, Pullman, WA
- ThP 389 **Separation of C18:1 Fatty acid Isomers using Cyclic Ion Mobility Mass Spectrometry;** Ahsan Hameed^{1,2}; Hailemariam Abrha Assress^{1,2}; Renny S Lan^{1,2}; Mario G Ferruzzi^{1,2}; Andrew J Morris^{1,3}; ¹Arkansas Children's Nutrition Center, Little Rock, AR; ²University of Arkansas for Medical Sciences, Little Rock, AR; ³Department of Pharmacology and Toxicology, University of Arkansas for Medical Sciences, Little Rock, Arkansas
- ThP 390 **Ion mobility of crosslinked peptide-RNA (oligo)nucleotides as a parameter for improved identification of crosslinks;** Sergei Moshkovskii¹; Olexandr Dybkov¹; Timo Sachsenberg²; Ralf Pflanz¹; Monika Raabe¹; Oliver Kohlbacher²; Henning Urlaub^{1,3}; ¹Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; ²University of Tübingen, Tübingen, Germany; ³University Medical Center Goettingen, Goettingen, Germany
- ThP 391 **SLIM Ion Mobility MS-Based Screening for Drugs of Abuse in Urine on a High-Throughput Development System;** Zongyuan Chen¹; Josh McBee¹; Miriam Fico¹;

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- Frederick G. Strathmann¹; Daniel Debord¹; ¹MOBILion Systems, Inc., Chadds Ford, PA
- ThP 392 **Amyloid formation of metabolites: Understanding the transformation of cysteine into amyloid-like fibrils and cystine crystal**; Thanh D Do¹; Damilola S. Oluwatoba¹; Miranda N. Limbach¹; ¹University of Tennessee, Knoxville, Knoxville, TN
- ThP 393 **Diagnostic Lipid Biomarkers discovery for Alzheimer's Disease using High-Resolution Ion Mobility Mass Spectrometry**; Orobola E. Olajide¹; Kimberly Y Kartowikromo¹; Junwei Wang¹; Yuyan Yi¹; Jingyi Zheng¹; Amal K Kaddoum¹; Ahmed M Hamid¹; ¹Auburn University, AUBURN, AL
- ThP 394 **Top/Middle-Down Characterization of α -Synuclein Glycoforms**; Kevin Jeanne Dit Fouque¹; Samuel A. Miller¹; Eldon Hard²; Matthew R. Pratt²; Francisco Alberto Fernandez Lima¹; ¹Florida International University, Miami, FL; ²University of Southern California, Los Angeles, CA
- ThP 395 **Rapid screening of Bispecific Antibodies and Antibody Impurities using In-source Collision Induced Unfolding coupled with IM-MS**; Ruwan Kurulugama¹; Christian Klein¹; Harsha P. Gunawardena²; ¹Agilent Technologies, Santa Clara, CA; ²Janssen Research & Development, Spring House, PA
- ThP 396 **Fast Separation and Quantitation of α -, iso- α - and β -acids via Differential Ion Mobility Spectrometry**; Emir Nazdrajić¹; Christian Ieritano^{1,2}; Scott Hopkins^{1,2,3}; ¹University of Waterloo, Waterloo, ON; ²Watermine Innovation, Waterloo, Ontario; ³Centre for Eye and Vision Research, Hong Kong, Hong Kong
- ThP 397 **Differentiation of isomeric, non-separable carbohydrates using Tandem Trapped Ion Mobility Spectrometry–Mass Spectrometry (tandem-TIMS/MS)**; Jusung Lee¹; Fanny C Liu¹; Christian Bleiholder¹; ¹Florida State University, Tallahassee, FL
- ThP 398 **Improving the annotation of bile acids in fecal samples using a Liquid Chromatography-Ion Mobility-High Resolution Mass Spectrometry method**; Dimitra Diamantidou^{1,2}; Christina Virgiliou^{1,2}; Olga Begou^{1,2}; Richard Seitz³; Carsten Baessmann⁴; Helen Gika^{1,2}; Georgios Theodoridis^{1,2}; ¹Aristotle University of Thessaloniki, Thessaloniki, Greece; ²Biomic AUTH, Center for Interdisciplinary Research and Innovation, Thessaloniki, Greece; ³Bruker Scientific, Billerica, MA; ⁴Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- ThP 399 **Imaging of Isomeric Metabolites in Mouse Brain with a nano-DESI timsTOF system**; Syeda Nazifa Wali¹; Lixue Jiang¹; Julia Laskin¹; ¹Purdue University, WEST LAFAYETTE, IN
- ThP 400 **In-depth identification and accurate quantification of mitochondrial and lysosomal crosstalk proteins**; Byoung-Kyu Cho¹; Young Ah Goo^{1,2,3}; ¹MTAC, MGI, Washington University School of Medicine in St. Louis, St. Louis, MO; ²Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine in St. Louis, St. Louis, MO; ³Department of Genetics, Washington University School of Medicine in St. Louis, St. Louis, MO
- ThP 401 **Confident identification of N-glycopeptides from standard glycoproteins using a cyclic ion mobility mass spectrometry system**; Sayantani Chatterjee¹; Joshua A. Klein²; Joseph Zaia^{1,2}; ¹Department of Biochemistry, Center for Biomedical Mass Spectrometry, Boston University Chobanian & Avedisian School of Medicine, Boston, MA; ²Bioinformatics Program, Boston University, Boston, MA
- ThP 402 **Influence of MS acquisition and integration parameters on isotope ratio determinations**; Huifang Yao¹; Haihong Zhou¹; David McLaren¹; Hao Chen²; Stephen Previs¹; ¹Merck & Co., Inc., Kenilworth, New Jersey; ²New Jersey Institute of Technology, Newark, NJ
- ThP 403 **Reimport of carbon from cytosolic and vacuolar sugar pools into the Calvin–Benson cycle explains photosynthesis labeling anomalies**; Yuan Xu¹; Thomas Wieloch²; Joshua A. M. Kaste¹; Yair Shachar-Hill¹; Thomas D. Sharkey¹; ¹Michigan State University, East Lansing, MI; ²Umeå University, Umeå, Sweden
- ThP 404 **LC-MS method to determine Coenzymes (CoA) Flux**; Vasanta Putluri¹; Abu Hena Mostafa Kamal²; Chandra Shekar Reddy Ambati²; Nagireddy Putluri²; ¹Baylor College of Medicine, Houston, TX; ²Baylor College of Medicine, Houston, Texas
- ThP 405 **Determination of mouse liver HSD17B13 protein half-life following metabolic labeling with deuterium oxide and quantitation with high resolution mass spectrometry**; Thomas Angel; GSK, King Of Prussia, PA
- ThP 406 **Fully labeled carbon-13 mice: an expanded view of the mammalian metabolome and its dynamics**; Annelaure Damont¹; Anaïs Legrand¹; Kathleen Rousseau¹; Laurent Bellanger²; Jean-Jacques Leguay³; Christophe Junot¹; François Fenaille¹; Eric Ezan¹; ¹CEA-INRA, Laboratoire Innovations en Spectrométrie de Masse pour la Santé (LI-MS), DRF / Institut Joliot / DMTS / SPI, MetaboHUB, CEA Saclay - Université Paris Saclay, Gif sur Yvette, France; ²Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), SPI, Bagnols-sur-Cèze, France; ³UMR 7265 CEA-CNRS-Université Aix Marseille, DRF/Institut de Biosciences et Biotechnologies d'Aix-Marseille (BIAM), plateforme PHYTOTECH, Cité des Energies, Saint-Paul-lez-Durance, France
- ThP 407 **A combined stable isotope infusion method to assess therapeutic efficacy in primary hyperoxaluria patients**; Dewi Van Harskamp¹; Sander F. Garrelfs²; Jaap W. Groothoff³; Michiel J.S. Oosterveld³; Johannes B. Van Goudoever⁴; Henk Schierbeek⁵; ¹Amsterdam UMC location University of Amsterdam, Department of Clinical Chemistry and Pediatrics, Laboratory Genetic Metabolic Diseases, Emma Children's Hospital, Amsterdam, Netherlands; ²Amsterdam UMC location University of Amsterdam, Department of Pediatric Nephrology, Emma Children's Hospital, Amsterdam, Netherlands; ³Amsterdam UMC location University of Amsterdam, Department of Pediatric Nephrology, Emma Children's Hospital, Amsterdam, Netherlands; ⁴Amsterdam UMC location University of Amsterdam, Department of Pediatrics, Emma Children's Hospital, Amsterdam, Netherlands; ⁵Amsterdam UMC location University of Amsterdam, Department of Pediatrics, Emma Children's Hospital, Amsterdam, Netherlands
- ThP 408 **Steady-state and dynamic operation of photorespiratory metabolism: integrating 13C metabolic flux analysis and pool size measurements**; Xinyu Fu¹; Berkley J Walker^{1,2}; ¹Department of Energy-Plant Research Laboratory, Michigan State University, East Lansing, MI; ²Department of Plant Biology, Michigan State University, East Lansing, MI
- ThP 409 **¹³CO₂ labeling for monitoring lipid biosynthesis in Lemna minor with MALDI-MSI**; Vy T Tat¹; Andrew E Paulson¹; Young Jin Lee¹; ¹Iowa State University, Ames, IA
- ThP 410 **Defining nutrient inputs that fuel glioblastoma metabolism in vivo using stable-isotope tracing metabolomics**; Andrew J Scott¹; Pietro Morlacchi²; Costas Lyssiotis¹; Daniel R. Wahl¹; ¹University of Michigan-Ann Arbor, Ann Arbor, MI; ²Agilent Technologies, Lexington, MA
- ThP 411 **A new StageTips method based on an innovative sorbent for fast and efficient peptide fractionation in proteomic studies**; Kaynoush Naraghi¹; Mana Shafaei²; Michel Arotçarena¹; Florine Hallez¹; Cerina Chhuon³; Chiara Guerrera³; Sami Bayoudh¹; ¹AFFINISEP, Le Houllme, France; ²Affinisep USA LLC, Miami, FL; ³INSERM - US24 SFR Necker Proteome, Paris, France
- ThP 412 **Optimization of solid phase extraction pretreatment for urinary DNA adductomics by high resolution mass spectrometry**; Alexandra Keidel¹; Carolina Möller²; Yuan-Jhe Chang³; Mu-Rong Chao^{3,4}; Jazmine Virzi²; Laura Deloso²; Theresa Evans-Nguyen¹; Chiung-Wen Hu⁵;

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- Marcus Cooke²; ¹Department of Chemistry, University of South Florida, Tampa, Florida; ²Oxidative Stress Group, Department of Molecular Biosciences, University of South Florida, Tampa, Florida; ³Department of Occupational Safety and Health, Chung Shan Medical University, Taichung, Taiwan; ⁴Department of Occupational Medicine, Chung Shan Medical University Hospital, Taichung, Taiwan; ⁵Department of Public Health, Chung Shan Medical University, Taichung, Taiwan
- ThP 413 **Deep proteomic coverage of human plasma in a fast, reproducible and easy-to-perform fashion: combining the novel ENRICH-iST workflow with fractionation; Sebastian H. Johansson¹; Katharina Limm¹; Katrin Hartinger¹; Kuan-Ting Pan¹; Nils A. Kulak¹; ¹PreOmics GmbH, Planegg/Martinsried, Germany**
- ThP 414 **The spatial proteome study based on micro-FFPETissues using LCMS sampling; Hao Chen; Beijing Genomics Institute, shenzhen, China**
- ThP 415 **Automated Sugaring-Out Assisted Liquid-Liquid Extraction and Determination of Neonicotinoids in Honey Samples using a Robotic Autosampler and LC-MS/MS Platform; Fred Foster¹; Megan Harper¹; Nicole Kfoury¹; Jaqueline Whitecavage¹; ¹Gerstel, Inc., Linthicum, MD**
- ThP 416 **Mature Fully Automated Peptide Mapping; Jason L. Richardson¹; Zhongqi Zhang¹; ¹Amgen, Thousand Oaks, CA**
- ThP 417 **Easy and Robust Automated Sample Preparation and Extraction for LC-MS/MS Bioanalytical Workflows; Jonathan Danaceau¹; Mary Trudeau¹; Meagan Callis¹; Steven Lai²; ¹Waters Corporation, Milford, MA; ²Waters corp, milford, MA**
- ThP 418 **The effects of DDM on proteomic data in routine usage; Xiaojing Yuan¹; Renata Moravcova²; Jason C. Rogalski¹; Leonard J. Foster²; ¹Proteomics Core Facility, UBC, Vancouver, BC; ²Department of Biochemistry and Molecular Biology, UBC, Vancouver, BC**
- ThP 419 **Advanced sample preparation in LC/MS bioanalysis using new solid phase extraction; Toshikazu Minohata¹; Ai Tsutsui¹; Haijuan An²; Keiko Shiren¹; Satoshi Yamaki¹; ¹SHIMADZU Corporation, Kyoto, Japan; ²Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd., Beijing, China**
- ThP 420 **β -Galactosidase spike-in as a strategy for normalisation in large-scale plasma DIA proteomics; Vineet Vaibhav^{1,2}; Samantha J Emery-Corbin^{1,2}; Megan Penno^{3,4}; Jumana M Yousef^{1,2}; Helena Oakley⁵; Jennifer J Couper⁵; Leonard C Harrison^{2,5}; John M Wentworth^{2,5}; Andrew I Webb^{1,2}; Laura F Dagley^{1,2}; ¹Advanced Technology and Biology Division, The Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia; ²Department of Medical Biology, University of Melbourne, Melbourne, Australia; ³Population Health Division, The Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia; ⁴Faculty of Health and Medical Sciences, The University of Adelaide, Adelaide, Australia; ⁵Faculty of Health and Medical Sciences, The University of Adelaide, Adelaide, Australia**
- ThP 421 **A complete and automated end-to-end sample preparation strategy for high-throughput and standardized proteomics with high sensitivity; Dorte B. Bekker-Jensen¹; Florian Harking²; Magnus Huusfeldt¹; Moritz Heusel¹; Lasse Falkenby¹; Jesper V. Olsen²; Nicolai Bache¹; ¹Evosep Biosystems, Odense, Denmark; ²University of Copenhagen, Copenhagen, Denmark**
- ThP 422 **Standardized, high-throughput platform for automated, rapid, and extensive plasma proteome characterization; Claudia Martelli¹; Fabian Wendt²; Andreas Schmidt³; Katrin Hartinger⁴; Gary Kruppa⁵; Nils A. Kulak⁴; Manuel Bauer²; ¹Bruker Switzerland AG, Fällanden, Switzerland; ²Tecan, Männedorf, Switzerland; ³Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ⁴PreOmics GmbH, Martinsried, Germany; ⁵Bruker S.R.O., Brno, Czech Republic**
- ThP 423 **Extraction and Quantitation of Per and Polyfluoroalkyl Substances (PFAS) in Bioanalytical Matrices Determined using UHPLC-MS/MS; Adam Senior¹; Kyle Bevan¹; Lee Williams¹; Geoff Davies¹; Alan Edgington¹; Helen Lodder¹; Russell Parry¹; Charlotte Hayes¹; Lucy Lund¹; Zainab Khan¹; Claire Desbrow¹; Dan Menasco¹; ¹Biotage GB Limited, Cardiff, United Kingdom**
- ThP 424 **Streamlined and semi-automated MS-based proteomics pipeline from protein extraction to real-time data analysis by coupling BeatBox, PreON and PaSER platforms; Measho Abreha¹; Jasmin Johansson²; Zehan Hu²; Jonathan Krieger³; Katharina Limm²; Katrin Hartinger²; Nils A. Kulak²; ¹PreOmics Inc., Islandia, NY; ²PreOmics GmbH, Planegg/Martinsried, Germany; ³Bruker Ltd, Milton, ON L9T 6P4**
- ThP 425 **Optimized proteolytic digestion fundamentals for maximizing protein identifications while reducing enzyme usage by an order of magnitude; Ivo A Hendriks¹; Michael L Nielsen¹; ¹Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, København, Denmark**
- ThP 426 **A comparison of silica SPE techniques - a novel hybrid composite versus traditional loose packed; James Edwards; Porvair Sciences, Wrexham, United Kingdom; J. G. Finneran, Vineland, NJ**
- ThP 427 **An optimized sample preparation workflow for rare cell subpopulation proteomics: from cell collection to sample injection; Christopher Kune¹; Sylvia Tielens²; Maximilien Fléron³; Dominique Baiwir³; Laurent Nguyen²; Gauthier Eppe¹; Gabriel Mazzucchelli^{1,3}; ¹Laboratory of Mass Spectrometry, MolSys Research Unit, University of Liège, Liège, Belgium; ²Laboratory of Molecular Regulation of Neurogenesis, GIGA-Stem Cells, University of Liège, Liège, Belgium; ³GIGA Proteomics Facility, University of Liège, Liège, Belgium**
- ThP 428 **Analysis of PFAS in Breast Milk: An Alternative Sample Prep; Tina Chambers¹; Jennifer Cottine Hitchcock¹; ¹Agilent Technologies, Santa Clara, CA**
- ThP 429 **Evaluation of Chemical Structure of SPE Reverse Phase Sorbents in StageTips on Total Number of Protein and Peptide Identifications; Michael Apsokardu¹; Xiaohui Zhang¹; Guotao Lu¹; ¹CDS Analytical, Oxford, PA**
- ThP 430 **A Three-in-One End-to-End Automated Sample Preparation and LC/MS Metabolomics, Lipidomics, and Proteomics Workflow for Plasma; Genevieve C. Van De Bittner¹; Karen E. Yannell¹; Mark Sartain¹; Wendi A. Hale²; Cate Simmermaker¹; Dustin Chang¹; ¹Agilent Technologies, Inc, Santa Clara, California; ²Agilent Technologies, Inc, Lexington, Massachusetts**
- ThP 431 **Innovation Development of Comprehensive Dimensional Profiling and Lossless Extraction Technology of the Multi-Residue Pesticides Analysis in TCM using LC-MS/MS; Bo Chen¹; Yue Song¹; Yu-Chia Lin²; Shan-An Chan³; ¹Agilent Technologies, Shanghai, China; ²Great Engineer Technology Crop., Taipei, Taiwan; ³Agilent Technologies, Taipei, Taiwan**
- ThP 432 **Building a universal proteomics sample preparation platform using low-cost liquid handling robotics and 3D-printing; Benedikt C. Clemens¹; Eric F Zaniewski¹; Johannes Kreuzer¹; Soroush Hajizadeh¹; Wilhelm Haas¹; ¹Massachusetts General Hospital, Boston, MA**
- ThP 433 **Classification of Bacterial Species from Whole Cell Lysates Using Two-Dimensional Tandem Mass Spectrometry and Open-Source Supervised Machine Learning; L. Edwin Gonzalez¹; Yanyang Hu²; Donna M Wang²; Eric T. Dziekonski²; R. Graham Cooks²; ¹Purdue University, West Lafayette, IN; ²Purdue University, WEST LAFAYETTE, IN**
- ThP 434 **Optimization of Lipid Extraction for Untargeted Lipidomic Analysis Using Liquid Chromatography/Mass Spectrometry; Ashraf M. Omar¹; Qibin Zhang^{1,2}; ¹Center for Translational Biomedical Research, University of North Carolina at Greensboro,**

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- North Carolina Research Campus, Kannapolis, NC;
²Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, NC
- ThP 435 **Elucidating the Lipidomic Dynamics of Lentiviral Production and Infection;** Joshua A Roberts¹; Elena Godbout²; Christopher Boddy³; Jean-Simon Diallo²; Jeffrey C Smith¹; ¹Carleton University, Ottawa, ON; ²Centre for Cancer Therapeutics, Ottawa Hospital Research Institute, Ottawa, ON; ³University of Ottawa, Ottawa, ON
- ThP 436 **Unlocking the Secrets of mRNA LNP Components Under Extreme Conditions with TIMS-TOF Technology;** Michael Girgis; George Mason University, Fairfax, VA
- ThP 437 **Evaluation of Aqueous-Acetonitrile Based Mobile Phase for Untargeted Analysis of Polar Metabolome and Lipidome;** Giorgis Isaac¹; Robert Plumb¹; ¹Waters Corporation, Milford, MA
- ThP 438 **Don't Be Ear-ritated: Kendrick Mass Defect-facilitated Determination of Triglycerides in Earwax;** Allix M. Coon¹; Gavin Setzen²; Rabi A. Musah¹; ¹University at Albany, State University of New York, Albany, NY; ²Albany ENT & Allergy Services, Albany, NY
- ThP 439 **Improved the detection and identification of labile lipids using Xevo™ G3 QTof Mass Spectrometer;** Nyasha C Munjoma¹; Steven Lai²; Lisa Reid¹; Jayne Kirk¹; Lee Gethings¹; Richard Lock¹; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters Corporation, Milford, MA
- ThP 440 **Discovery Lipidomics and Mapping of Exogenous Fatty Acid Incorporation into the HeLa Lipidome Using LC-IMS/MS and LC-IMS/MS/MS;** Johannes Morstein¹; Andrew Baker²; ¹University of California San Francisco, San Francisco, CA; ²Waters, Inc., Pleasanton, CA
- ThP 441 **How Acute Exercise Alters Rat's Lipidomic Profile of Liver;** David A Gaul¹; Samuel G Moore¹; Xueyun Liu²; Kristal Maner-Smith²; Eric Ortlund²; Karyn A Esser³; Laurie J Goodyear⁴; Facundo M Fernandez¹; ¹Georgia Institute of Technology, Atlanta, GA; ²Emory University, Atlanta, GA; ³University of Florida, Gainesville, FL; ⁴Harvard Medical School, Boston, MA
- ThP 442 **Variations in Lipid Profiles in the Serum Coronas Produced around Liposomal Drugs with Different Surface Properties;** Gwi Ju Jang¹; Heeju Joung¹; Sang Yun Han¹; ¹Department of chemistry, Gachon University, Seongnam, South Korea
- ThP 443 **Untargeted 2DxLC-Mass Spectrometry using SWATH-DIA-Based Workflow for the Characterization of Lipid Profiles in Plasma Samples;** Laura Gisela González Iglesias¹; Gerard Hopfgartner¹; Renzo Picononi²; Guenter Boehm²; ¹LSMS, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; ²CTC Analytics AG, Zwingen, Switzerland
- ThP 444 **Comprehensive lipidome profiling facilitates the discovery of targetable metabolic vulnerabilities in Group 3 medulloblastoma;** Jeremy K. Chan¹; William D. Gwynne¹; Andrew T. Quaille¹; J. Rafael Montenegro-Burke¹; ¹Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON
- ThP 445 **Untargeted lipidomics analyses of exosomes from malaria parasite-infected red cells;** Sina Feizbakhsh Bazargani¹; Timothy Hamerly²; Borja Lopez-Gutierrez²; Rhoel R Dinglasan²; Timothy J. Garrett²; ¹University of Florida, Gainesville, FL; ²University of Florida, Gainesville, Florida
- ThP 446 **Lipid composition of serum-derived small extracellular vesicles could discriminate rectal cancer patients with different status of regional lymph node metastasis;** Lukasz Marczak¹; Katarzyna Dubkiewicz¹; Marcin Zeman²; Monika Pietrowska²; Anna Wojakowska¹; ¹Institute of Bioorganic Chemistry Polish Academy of Sciences, Poznan, Poland; ²Maria Skłodowska-Curie National Research Institute of Oncology, Gliwice Branch, Gliwice, Poland
- ThP 447 **Lipidomic Analysis of Human Serum of Pancreatic Cancer Patients with Focus on Less Abundant Lipid**
- Classes by HILIC-UHPLC/MS;** Ondřej Peterka¹; Alessandro Maccelli¹; Robert Jirásko¹; Zuzana Vaňková¹; Jakub Idkowiak¹; Denise Wolrab¹; Roman Hrstka²; Michal Holčápek¹; ¹University of Pardubice, Pardubice, Czech Republic; ²Masaryk Memorial Cancer Institute, Brno, Czech Republic
- ThP 448 **The inhibition of TGFβ changed the profiles of collagen crosslinks and lipids in tumor;** Qingling Li¹; Alessandra Castiglioni²; Yagai Yang²; Shannon Turley²; Rafael Cubas²; Wendy Sandoval²; ¹Genentech, SSF; ²Genentech Inc, South San Francisco, CA
- ThP 449 **Development of an MRM based phospholipid profiling method in human plasma using an inert C18 column;** Masaki Yamada¹; Naoko Nagano¹; Yutaka Umakoshi¹; ¹SHIMADZU Corporation, Kyoto, Japan
- ThP 450 **High-throughput UHPLC-TIMS-based lipidomics: Sub-5 min screening of plasma, cells, stool and tissues;** Eduardo Sommella¹; Fabrizio Merciai¹; Pietro Campiglia¹; Erica Forsberg²; ¹University of Salerno, Fisciano (SA), Italy; ²Bruker Daltonics, San Jose, CA
- ThP 451 **Inorganic arsenic treatments alter lipidomic profiles of Escherichia coli;** Brett T Sather¹; Hunter Fausset¹; Scott Spurzem¹; Garrett Gill¹; Cole Kayser¹; Anya Knowlton¹; Georgia Eastham¹; Sydney Peterson¹; Brian Bothner¹; ¹Montana State University, Bozeman
- ThP 452 **Lipidomics on a High Fat Diet mouse model indicate alterations in lipid metabolism upon aerobic exercise and calories restriction;** Thomai Mouskeftara^{1,2}; Christina Virgiliou^{1,2}; Ioannis I. Moustakas³; Eric Halls⁴; Carsten Baessmann⁵; Helen Gika¹; ¹Aristotle University of Thessaloniki, Thessaloniki, Greece; ²Bionic AUTH, Center for Interdisciplinary Research and Innovation, Thessaloniki, Greece; ³Medical School, National and Kapodistrian University of Athens, Athens, Greece; ⁴Bruker Daltonics, Billerica, MA; ⁵Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- ThP 453 **Lipidomics analysis reveals changes in the regulation of lipid metabolism in a surgical bone defect model;** Dilrukshika S. W. Palagama¹; Matthew J Kwiatkowski¹; Phillip M Rzeczycki¹; Thomas A Owen¹; Maria I Morano¹; Miguel A Gijón¹; Paul D Kennedy¹; Stephen D Barrett¹; ¹Cayman Chemical Company, Ann Arbor, MI
- ThP 454 **Coupling MaxPeak HPS UHPLC and PASEF-enabled lipidomics to maximize performance for multimodal analysis of small human biopsies;** Madeline E Colley^{1,2}; Katerina V Djambazova^{2,3}; Lukasz G Migas⁴; Martin Dufresne^{1,2}; Jamie L. Allen^{1,2}; Angela R. S. Kruse^{1,2}; Richard M Caprioli^{1,2,5,6,7}; Raf Van De Plas^{1,2,4}; Jeffrey M Spraggins^{1,2,3,7}; ¹Vanderbilt University, Department of Biochemistry, Nashville, Tennessee; ²Mass Spectrometry Research Center, Vanderbilt University, Nashville, Tennessee; ³Department of Cell and Developmental Biology, Vanderbilt University, Nashville, Tennessee; ⁴Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; ⁵Department of Medicine, Vanderbilt University, Nashville, Tennessee; ⁶Department of Pharmacology, Vanderbilt University, Nashville, Tennessee; ⁷Department of Chemistry, Vanderbilt University, Nashville, Tennessee
- ThP 455 **4D-lipidomics for the in-depth characterization of cardiolipins in Barth Syndrome patient hearts using VIP-HESI and timsTOF mass spectrometry;** Sven Wolfgang Meyer¹; Yorrick R.J. Jaspers²; Bauke V. Schomakers^{2,3}; Jan Bert Van Klinken^{2,3,4}; Eric Wever^{2,3}; Stephan Kemp²; Frédéric M. Vaz^{2,3}; Riekelt H. Houtkooper²; Michel Van Weeghel^{2,3}; ¹Bruker Daltonics GmbH & Co. KG, Bremen, Germany; ²Laboratory Genetic Metabolic Diseases, Amsterdam UMC, University of Amsterdam, Amsterdam Gastroenterology Endocrinology Metabolism, Amsterdam, Netherlands; ³Core Facility Metabolomics, Amsterdam UMC, Amsterdam, Netherlands; ⁴Department of Human Genetics, Leiden University Medical Center, Leiden, Netherlands

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- ThP 456 **Establishment of a global metabolomics method for *Arabidopsis thaliana* using high-sensitivity MS/MS on the ZenoTOF 7600 system;** Jinmei Chen¹; Dandan Si²; Zhimin Long¹; Lihai Guo²; ¹SCIEX, Shanghai, China; ²SCIEX, Beijing, China
- ThP 457 **Classification of Beef Using Metabolomics;** Zhentian Lei¹; Saurav Sarma²; Carol Lorenzen³; Jade Cooper⁴; Lloyd Sumner⁵; ¹University of Missouri, Columbia, MO; ²Bayer Crop Science, St. Louis, MO; ³Oregon State University, Corvallis, OR; ⁴Texas A&M University, College Station, TX; ⁵University of Missouri-Columbia, Columbia, MO
- ThP 458 **Advantages of a novel high resolution accurate mass analyzer for metabolite identification in untargeted metabolomics studies;** Siegrun Mohring¹; Bashar Amer²; Susan Bird²; Nicolaie Eugen Damoc¹; Martin Zeller¹; Alexander Tiegel¹; ¹Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ²Thermo Fisher Scientific, San Jose, California
- ThP 459 **A Multi-Omics Approach to Investigate Interactions between *Elizabethkingia anophelis* and Zika Virus;** Junyao Wang¹; Omme Fatema Sultana¹; Maria Onyango¹; Yehia Mechref¹; ¹Texas Tech University, Lubbock, TX
- ThP 460 **Development of Chemical Isotope Labeling LC-Orbitrap-MS for Comprehensive Analysis of small peptides;** Zhan Cheng¹; Liang Li¹; ¹University of Alberta, Edmonton, AB
- ThP 461 **Targeted and untargeted metabolomics of mucopolysaccharidoses model in mouse liver by LC-MS/MS;** Nathan Ghafari¹; Iskren Menkovic²; Pamela Lavoie²; Michel Boutin²; Christiane Auray-Blais²; Lekha Sleno³; ¹University of Quebec in Montreal, Montreal, QC; ²Department of Pediatrics, Division of Medical Genetics, Faculty of Medicine and Health Sciences, Sherbrooke University, Sherbrooke, QC; ³University of Quebec in Montreal (UQAM), Chemistry department, Montreal, QC
- ThP 462 **Utilizing Tandem Mass Spectrometry and Computational Methods to Elucidate Fragmentation Mechanisms for Kynurenine Metabolites;** Madisyn Hayes¹; Esther Mbuna¹; Jaya Paudel¹; Dr. Benjamin Bythell¹; ¹Ohio University, Athens, OH
- ThP 463 **Non-targeted metabolomics investigation suggests female is more vulnerable to sub-chronic variable stress leading to depression in association with insulin resistance;** Seulgi Kang¹; Boyeon Bae¹; Woonhee Kim²; Jimin Nam²; Ke Li¹; Yua Kang¹; Chihye Chung²; Jeongmi Lee¹; ¹Sungkyunkwan University, Suwon, South Korea; ²Konkuk University, Seoul, South Korea
- ThP 464 **Understanding the impact of sourdough starter microbiomes on bread quality;** Eva Keohane¹; Jacqueline Chaparro¹; Josephine Wee²; Charlene Van Buiten¹; Jessica Prenni¹; ¹Colorado State University, Fort Collins, CO; ²Penn State University, Centre County, Pennsylvania
- ThP 465 **Impact of *Toxoplasma gondii* acute and chronic infection on organ metabolism in IL-1R^{-/-} and WT mice;** Mahbobeh Lesani¹; Tzu-Yu Feng²; Sarah E. Ewald²; Laura-Isobel McCall^{3,4}; ¹University of Oklahoma, Norman, OK; ²University of Virginia, Charlottesville, VA; ³University of Oklahoma, Department of Microbiology and Plant Biology, Norman, OK; ⁴University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK
- ThP 466 **A Novel Screening Approach for Comparing LC-MS Reversed-Phase and HILIC Methods for Separations in Biological Matrices Using Amino Acid Examples;** Conner McHale¹; Taylor Harmon¹; ¹Advanced Materials Technology, Wilmington, DE
- ThP 467 **Metabolic profile variation of *Fragaria annanassa* induce by *Arthospora platensis* addition, under condition of nutritional stress;** Candy Andreina Montaña-Pérez^{1,2}; Cecilia-Rocio Juárez-Rosete¹; Juan José Ordaz-Ortiz³; Javier-German Rodríguez-Carpena²; Gabriela Ávila-Villarreal^{2,4}; ¹Maestría Interinstitucional en Agricultura Protegida, CONACyT, Unidad Académica de Agricultura, Universidad Autónoma de Nayarit, Tepic, Mexico; ²Unidad Especializada en I+D+i Calidad de Alimentos y Productos Naturales, Centro Nayarita de Innovación y Transferencia de Tecnología A.C., Tepic, Mexico; ³Unidad de Genómica Avanzada, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, CINVESTAV, (LANGEBIO), Irapuato, Mexico; ⁴Unidad Académica de Ciencias Químico Biológicas y Farmacéuticas, Universidad Autónoma de Nayarit, Tepic, Mexico
- ThP 468 **Metabolomics of Colorectal Cancer for Human Serum Screening;** Kinjal Bhatt¹; Marie-Alice Meuwis²; Edouard Louis²; Pierre-Hugues Stefanuto¹; Jean Francois Focant¹; ¹University of Liege, Liege, Belgium; ²Liege University Hospital, Liege, Belgium
- ThP 469 **System suitability testing of LC-IMS-HRMS for metabolomics applications;** Sven Wolfgang Meyer¹; Ilmari Krebs¹; Stefan Harsdorf¹; Patrick Groos¹; Jonas Wloka¹; Erica Forsberg¹; Matthew R. Lewis¹; ¹Bruker Daltonics GmbH & Co. KG, Bremen, Germany
- ThP 470 **PlantMASST: a mass spectrometry tool for mining public datasets from plants;** Paulo Wender Portal Gomes¹; Helena Mannocho-Russo¹; Simone Zuffa¹; Robin Schmid¹; Andrés Mauricio Caraballo-Rodríguez¹; Pieter C Dorrestein¹; ¹Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, San Diego, California
- ThP 471 **A metabolomics approach using Simultaneous Quantitation and Discovery (SQUAD) on high resolution accurate mass full MS1 level;** Bashar Amer¹; Christian Klaas²; Catharina Crone²; Siegrun Mohring²; Rahul Deshpande¹; Claire Dauly²; Thomas Moehring²; Susan S. Bird¹; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- ThP 472 **Mass spectrometry analysis of the effect of hemin on *Pseudomonas aeruginosa* alkyl quinolone production;** Daniel J Breiner¹; Rachel Neve²; Vanessa V. Phelan³; ¹CU Anschutz Skaggs School of Pharmacy and Pharmaceutical Science, Aurora, CO; ²University of Massachusetts Medical School, Worcester, MA; ³University of Colorado Anschutz Medical Campus, Aurora, CO
- ThP 473 **Integrated analysis of LC/MS and GC/MS data in NASH and NAFLD model mice;** Yutaka Umakoshi¹; Tsutomu Matsubara²; Chiho Kadono²; Yuki Sakamoto¹; ¹SHIMADZU Corporation, Kyoto, Japan; ²Osaka Metropolitan University, Osaka, Japan
- ThP 474 **An Innovation Solution of Functional Metabolomics Reveal the Central role of Pentose Phosphate Pathway in Resident Thymic Macrophages;** Tsung-Lin Tsai¹; Chia-Lin Hsu¹; Yue Song²; Dai-Yong Huang³; Shan-An Chan⁴; Yanan Yang⁵; ¹Institute of Microbiology and Immunology, National Yang Ming Chiao Tung University, Taipei, Taiwan; ²Agilent Technologies, Shanghai, China; ³Agilent Technologies, Inc, Guangdong, China; ⁴Agilent Technologies, Taipei, Taiwan; ⁵Agilent Technologies, Santa Clara, CA
- ThP 475 **Feature-based molecular networking revealed *Jasminum sambac* cell extract as a powerful mixture of antioxidant metabolites;** Sara Ceccacci¹; Adriana De Lucia²; Assunta Tortora²; Antonio Colantuono²; Gennaro Carotenuto²; Annalisa Tito²; Maria Chiara Monti¹; ¹Department of Pharmacy, University of Salerno, Fisciano, Italy; ²Arterra Bioscience SpA, Naples, Italy
- ThP 476 **Characterization of the diurnal pattern of exhaled volatile fatty acids and enteric methane emissions of dairy cows;** Stamatios Giannoukos¹; Zakirul Islam²; Susanna Räisänen²; Kai Wang²; Xiaoqi Ma²; Fabian Wahl³; Renato Zenobi¹; Mutian Niu²; ¹ETH Zurich, Zurich, Switzerland; ²ETH Zurich, Zurich, Switzerland; ³Agroscope, Bern, Switzerland
- ThP 477 **Investigating systemic gut microbiome derived metabolites from IL18^{-/-} mice as potential mechanisms in health and disease;** Emily G Armitage¹; Alan Barnes¹;

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- Nicholas Groth Merrild²; J Miotla Zarebska²; Neil Loftus¹; Jonathan Swann³; Tonia L Vincent²; ¹*Shimadzu Corporation, Manchester, United Kingdom*; ²*Kennedy Institute of Rheumatology, University of Oxford, Oxford, United Kingdom*; ³*School of Human Development and Health, Faculty of Medicine, University of Southampton, Southampton, United Kingdom*
- ThP 478 **Reproducibility Analyses of Metabolomic Data**; Xinjian Yan¹; Stephen E. Stein¹; ¹*National Institute of Standards and Technology, Gaithersburg, MD*
- ThP 479 **Evaluation of a UPLC zwitterionic HILIC stationary phase for deep coverage and high throughput metabolomics**; Rebecca E. Jones¹; Lia Ficaró¹; Tori Rodrick¹; Manor Askenazi²; Yik Siu¹; Thomas H. Walter³; Kerri M. Smith³; Jonathan Turner³; Drew R. Jones¹; ¹*NYU Langone Health, New York*; ²*Biomedical Hosting LLC, Arlington, MA*; ³*Waters Corporation, Milford, Milford, MA*
- ThP 480 **Untargeted metabolomic analysis of acute lead exposure to Danio rerio embryos using LC-MS/MS**; Gwendolyn Cooper¹; Tyler K. Hunt-Smith²; Hunter Fausset¹; Christa S. Merzdorf²; Brian Bothner¹; ¹*Department of Chemistry and Biochemistry, Montana State University, Bozeman, Montana*; ²*Department of Microbiology and Immunology, Montana State University, Bozeman, Montana*
- ThP 481 **Exploring the Effect of Yeast Strain and Hop Addition Time on the Metabolomics of Beer**; Ciara Myer¹; Eric D. Tague¹; Christopher Bolcato¹; Amirmansoor Hakimi¹; Lance Shaner²; Laura Burns²; ¹*Thermo Fisher Scientific, San Jose, California*; ²*Omega Yeast, Chicago, Illinois*
- ThP 482 **Understanding early metabolic response of *Saccharomyces cerevisiae* to different oxidants using quantitative metabolomics with Isotopic Ratio Outlier Analysis (IROA)**; Debasish Ghosh¹; Felice A. De Jong²; Chris Beecher²; Vladimir Shulaev¹; ¹*University of North Texas, Denton, TX*; ²*IROA Technologies, Chapel Hill, NC*
- ThP 483 **Simultaneous Quantitation and Discovery (SQUAD) metabolomics: an intelligent combination of targeted and untargeted workflows using a novel mass spectrometer**; Bashar Amer¹; Siegrun Mohring²; Nicolaia Eugen Damoc²; Tabiwang N. Arrey²; Rahul Ravi Deshpande¹; Daniel Hermanson¹; Thomas Moehring²; Susan Bird¹; ¹*Thermo Fisher Scientific, San Jose, California*; ²*Thermo Fisher Scientific, Bremen, Germany*
- ThP 484 **Simultaneous Quantitation and Discovery (SQUAD) metabolomics workflow implementing parallel analysis on Thermo Ascend Tribrid instrument**; Bashar Amer¹; Jingjing Huang¹; David Bergen¹; Rahul Ravi Deshpande¹; Vlad Zabrouskov¹; Thomas Moehring²; Susan Bird¹; ¹*Thermo Fisher Scientific, San Jose, California*; ²*Thermo Fisher Scientific, Bremen, Germany*
- ThP 485 **Evaluating the metabolic function of LuxS and Autoinducer-2 in *Escherichia Coli***; Lindsay P Brown¹; Shawn R. Campagna¹; ¹*University of Tennessee Knoxville Chemistry Dept., Knoxville, TN*
- ThP 486 **Elucidating the progressive multiorgan metabolic response in the setting of mitochondrial myopathies using combined omics and in-vivo stable isotope tracing**; Dawson Miller¹; Steven S Gross¹; Marilena D'aurelio¹; Qiuying Chen²; ¹*Weill Cornell Medicine, New York, NY*; ²*Cornell University Medical College, New York, NY*
- ThP 487 **Differentiating Lung Tumor Biology in Metabolomes using Matched Flash Frozen and Fixed Tissues**; Vanessa Y. Rubio¹; Hayley D. Ackerman¹; John H. Lockhart¹; Nicole R. Hackel¹; Elsa R. Flores¹; John M Koomen¹; ¹*Moffitt Cancer Center, Tampa, FL*
- ThP 488 **Metabolomics investigation of poly-l-lysine induced cytotoxicity**; Vahid Jahed^{1,2}; Kristine Aunina¹; Liva Vita Kaufmane¹; Fatemeh Rastegar Adib¹; Dagnija Loca^{1,2}; Kristaps Klavins^{1,2}; ¹*Riga Technical University, Riga, Latvia*; ²*Baltic Biomaterials Centre of Excellence, Headquarters at Riga Technical University, Riga, Latvia*
- ThP 489 **A Simultaneous Quantitation and Discovery (SQUAD) Tribrid method template combining Ion Trap and Orbitrap analysis**; Sunandini Yedla¹; Brandon Bills¹; Bashar Amer¹; Rahul Deshpande¹; Susan Bird¹; Vlad Zabrouskov¹; Elys Rodriguez²; Uri Keshet²; Oliver Fiehn²; ¹*ThermoFisher Scientific, San Jose, CA*; ²*UC Davis, Davis, CA*
- ThP 490 **Investigating the Impact of Flame Retardants on Stem Cell Differentiation by Untargeted Metabolomics**; Whitney L Stutts¹; Yu-Chun Chiu¹; Melissa Gronske¹; Seth W. Kullman¹; ¹*North Carolina State University, Raleigh, NC*
- ThP 491 **Nitrilotriacetic acid-conjugated magnetic nanoparticle affinity probe-based mass spectrometry for porphyrin profiling**; Elias Gizaw Mernie¹; Mei-Chun Tseng^{2,3}; Rofeamor P Obena¹; Fu-Lien Huang⁴; Tzu-Ming Liu⁵; Yu-Ju Chen^{1,6}; ¹*Institute of Chemistry, Academia Sinica, Taipei, Taiwan*; ²*Institute of Chemistry, Academia Sinica, Taipei, Taiwan*; ³*Department of Chemistry, Taipei, Taiwan*; ⁴*Institute of Biomedical Engineering, National Taiwan University, Taipei, Taiwan*; ⁵*Institute of Translational Medicine, Faculty of Health Sciences, University of Macau, Macau, China*; ⁶*Department of Chemistry, National Taiwan University, Taipei, Taiwan*
- ThP 492 **Interfacing chromatographic, mass spectrometry, and ionization techniques for a better profiling of endogenous and exogenous metabolites in human milk**; Aliyah A. Remoroza¹; Yamil Simón-Manso²; Concepcion A. Remoroza²; William E. Wallace²; Stephen E. Stein²; Chengpeng Chen¹; ¹*University of Maryland - Baltimore County, Baltimore, MD*; ²*National Institute of Standards and Technology, Gaithersburg, MD*
- ThP 493 **Identification of Xenobiotic Biotransformation Products Using Mass Spectrometry-based Metabolomics Integrated with a Structural Elucidation Strategy by Assembling Fragment Signatures**; Yuan-Chih Chen¹; Pao-Chi Liao¹; ¹*National Cheng Kung University, Tainan, Taiwan*
- ThP 494 **Dynamic 13C isotopic labeling and metabolic flux analysis of two fast-growing cyanobacteria: a study with SWATH tandem mass spectrometry**; Pramod P Wangikar¹; Damini Jaiswal¹; Minal Nenwani¹; ¹*Indian Institute of Technology Bombay, Mumbai, India*
- ThP 495 **Metabolite structure elucidation and analysis enabled by a curated microbial biotransformation screen**; Chris J Brown¹; Yelena Adelfinskaya²; Yue Fu^{2,3}; Jesse Balcer²; Krishna Kuppanan²; Yannick Djoumbou Feunang²; Matt Chase²; Elizabeth Ibwe²; Serge Fotso²; Paul Graupner²; David Robbins¹; Jeffrey Gilbert²; ¹*Corteva Agrisciences, Indianapolis, IN*; ²*Corteva Agriscience, Indianapolis, IN*; ³*Purdue University, Lafayette, IN*
- ThP 496 **Benchmarking the relationship between spectral and chemical similarity in the context of chemical classes and molecular networking**; Yasin El Abiead¹; Wout Bittremieux²; Robin Schmid³; Simone Zuffa¹; Justin J Van Der Hoof⁴; Mingxun Wang⁵; Pieter C Dorrestein¹; ¹*Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, San Diego, CA*; ²*Campus Middelheim, University of Antwerp, Antwerpen, Belgium*; ³*IOCB Prague, Prague, Czech Republic*; ⁴*Wageningen University, Wageningen, Netherlands*; ⁵*University of California Riverside, Riverside, CA*
- ThP 497 **Investigation of the zearalenone metabolism using Electrochemistry-MS: Electrochemical vs. in vivo and in vitro approaches**; Jean-Pierre Chervet¹; Boguslaw Buszewski²; Malgorzata Szultka-Mlynska²; ¹*Antec Scientific, Alphen a/d Rijn, Netherlands*; ²*Nicolaus Copernicus University, Faculty of Chemistry, Torun, Poland*
- ThP 498 **Novel real-time acquisition logic to prevent fragmentation of uninformative precursors**; Pelle Simpson¹; Nikolas Kessler²; Christopher L. Clark³; Heiko Neuweger¹; ¹*Enveda Biosciences, Boulder, CO*; ²*Bruker Daltonics GmbH & Co. KG, Bremen, Germany*; ³*Bruker Scientific, LLC, Billerica, MA*

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- ThP 499 **Topic modelling improves accuracy of feature assignment in untargeted metabolomic analysis of the cancer microbiome**; Devanand M. Pinto¹; Andrew Leslie¹; Tracy McGaha²; Kenneth Chisholm¹; ¹NRC, Halifax, NS; ²Princess Margaret Cancer Centre, University Health Network, Toronto, ON
- ThP 500 **Real time library search for the confident annotation of compound classes on Thermo Ascend Tribrid instrument**; Rahul Ravi Deshpande¹; Bashar Amer¹; Jingjing Huang¹; David Bergen¹; Thomas Moehring²; Susan Bird¹; ¹Thermo Fisher Scientific, San Jose, California; ²Thermo Fisher Scientific, Bremen, Germany
- ThP 501 **Phyto-metabolomics of *Phlogacanthus curviflorus* by using an integrative LC-ESI-QTOF-MS/MS and GC/Q-TOF-MS approach: Evaluation of Antioxidant activity and enzyme inhibition potential**; Srikanth Ponneganti; National Institute of Pharmaceutical Education and Research Guwahati (NIPER-G), Guwahati, India
- ThP 502 **Multi-omics Profiling Shows Acetyl-CoA Carboxylase Inhibition Rewires T cell Lipidome**; Diane Wallace¹; Jess Thaxton^{2,3}; Brian P. Risenberg²; Katie Hurst²; Elizabeth Hunt^{2,4}; Brandie Ehrmann¹; ¹Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; ²Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC; ³Department of Department of Cell Biology & Physiology, University of North Carolina at Chapel Hill, Chapel Hill, NC; ⁴Department of Department of Cell Biology & Physiology, University of North Carolina at Chapel Hill, Chapel Hill, NC
- ThP 503 **Application of A UPLC-QTOF-MS/MS Metabolomics Approach to Identify Yellow Rice Wine with Different Aging Times**; Huimin Chen¹; Jiangang Hu²; Zong Yang³; Bingjie Liu³; Lihai Guo³; ¹SCIEX, Nanjing, China; ²Shaoxing Testing Institute of Food and Drug, Shaoxing, China; ³SCIEX, Shanghai, China
- ThP 504 **Untargeted metabolomics of human urine from the hPOP consortium: profiling variations by gender, age, body mass index, ethnicity and nutrition**; Myriam Mireault¹; Lekha Sleno¹; ¹University of Quebec in Montreal (UQAM), Chemistry department, Montreal, QC
- ThP 505 **Comprehensive metabolomic analysis of single-spheroids based on chemical isotope labeling liquid chromatography-mass spectrometry**; Cyrene Catenza¹; Liang Li^{1,2}; ¹University of Alberta, Edmonton, AB; ²The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta
- ThP 506 **Creation of the HoneyBee Metabolomics DataBase (HBDB)**; Armando Alcazar Magana¹; Sofia Colmenares¹; Jason C. Rogalski^{1,2}; Peter Awram³; Leonard J. Foster⁴; ¹Life Sciences Institute, UBC, Vancouver, British Columbia; ²UBC, Vancouver, BC; ³Authentic Food Solutions, Vancouver, British Columbia; ⁴Department of Biochemistry and Molecular Biology, UBC, Vancouver, BC
- ThP 507 **Development of Robust and Sensitive Chemical Isotope Labeling (CIL) LC-MS for Metabolomic Profiling of One Microliter of Human Serum**; Xian Luo¹; Liang Li²; ¹The Metabolomics Innovation Centre, Edmonton, AB; ²University of Alberta, Edmonton, AB
- ThP 508 **Enniatins and beauvericin emerging mycotoxins affect pigs' metabolome**; Emilien L Jamin^{1,2}; Justin Oules^{1,2}; Jean-François Martin^{1,2}; Barbara Novak³; Dian Schatzmayr³; Isabelle P Oswald¹; Oliver Puel¹; Philippe Pinton¹; ¹Toxalim (Research Center in Food Toxicology), Toulouse university, INRAE, ENVT, INP-Purpan, Toulouse, France; ²MetaboHUB-MetaToul, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France; ³DSM - BIOMIN Research Center, Technopark 1, Tulln, Austria
- ThP 509 **Genome mining and untargeted metabolomics to discover secondary metabolites involved in ectomycorrhizal fungal interactions**; Sameer Mudbhari^{1,2}; Manasa R. Appidi^{1,2}; Rytas Vilgalys³; Robert L. Hettich^{1,2}; Lotus Lofgren³; Paul E. Abraham^{1,2}; ¹The University of Tennessee, Knoxville, Tennessee; ²Oak Ridge National Laboratory, Oak Ridge, TN; ³Duke University, Durham, NC
- ThP 510 **Longitudinal multi-omics characterization of propyl gallate-mediated nephrotoxicity in beagles**; Nathaly Reyes Garces¹; Weiwen Sun¹; Si Mou¹; Tim Hummer²; Xuejun Peng³; Alvaro Sebastian Vaca⁴; Erica Forsberg⁴; Matt Willetts⁵; Anton I. Rosenbaum¹; Kevin Contrepois¹; ¹AstraZeneca, South San Francisco, CA; ²AstraZeneca R&D, Gaithersburg, Maryland; ³Bruker Scientific, San Jose, CA; ⁴Bruker, San Jose, CA; ⁵Bruker Scientific, Billerica, MA
- ThP 511 **Development of an Ion Chromatography Mass Spectrometry Platform and Spectral Library for Cancer Metabolomics**; Sara A Martinez¹; Lin Tan¹; Bao Tran¹; John Weinstein¹; Philip Lorenzi¹; ¹The University of Texas MD Anderson Cancer Center, Houston, TX
- ThP 512 **Signal Response Evaluation Cleans Untargeted Mass Spectrometry Data to Improve Data Interpretability**; Kirsten E Overdahl¹; Alan K Jarmusch¹; ¹National Institute of Environmental Health Sciences, Research Triangle Park, NC
- ThP 513 **A New Methodology Approach for Metabolomics Analysis of Rumen**; Kaitlyn M Melo¹; Janet Li¹; Sang Weon Na²; Mi Zhou²; Le Luo Guan²; Liang Li¹; Shuang Zhao¹; ¹The Metabolomics Innovation Centre, University of Alberta, Edmonton, AB; ²Department of Agricultural, Food and Nutritional Science, University of Alberta, Edmonton, AB
- ThP 514 **Enhancing the mobility resolution for co-eluting compound classes during plasma characterisation using multi-sequence IMSn acquisitions**; Adam M King¹; Christopher Jurtschenko²; Dale A. Cooper-Shepherd³; Martin Palmer³; Darren Hewitt³; Emma Marsden-Edwards³; ¹Waters corporation, Wilmslow, United Kingdom; ²Waters, Milford, MA; ³Waters Corporation, Wilmslow, United Kingdom
- ThP 515 **Secretory response of *Aspergillus niger* IOC 4687 subjected to copper stress**; Silas De Almeida Perdigão Cota De Almeida¹; Enrique Eduardo Rozas¹; Claudio Augusto Oller Nascimento¹; Meriellen Dias¹; Maria Anita Mendes¹; ¹Dempster MS Lab, Chemical Engineering Department of Polytechnic School of University of São Paulo (USP), São Paulo, Brazil
- ThP 516 **Production and Characterization of Hydrothermal Extracts of the Needles from Four Conifer Tree Species**; Omolara O. Mofikoya¹; Eemeli Eronen¹; Marko Mäkinen¹; Janne Jänis¹; ¹University of Eastern Finland, Department of Chemistry, Joensuu, Finland
- ThP 517 **Biochemical phenotyping of null alleles in human induced pluripotent stem cell-derived cell lineages: integrating genetics with metabolomics**; Maheshwor Thapa¹; Shujian Zheng¹; Nelio Oliveira¹; Arti Taggar^{1,2}; Amnah Siddiqi¹; Minghao Gong¹; Anahita Amiri¹; Justin McDonough¹; Bill Skarnes^{1,2}; Paul Robson^{1,2}; Shuzhao Li^{1,2}; ¹The Jackson Laboratory, Farmington, CT; ²University of Connecticut School of Medicine, Farmington, CT
- ThP 518 **GC-MS Metabolomic Profiling of Honey Samples from Zambia and Botswana for Geographical Origin Classification**; Kwenga F Sichilongo¹; Tumelo Padiso¹; Bonang B Nkoane¹; Godiraone Tatolo¹; Ogaufi Modisane¹; ¹University of Botswana, Gaborone, Botswana
- ThP 519 **Differences in metabolic profiles of patients with heart failure using high resolution GC/Q-TOF**; Sofia Nieto¹; Luis Valdiviez²; Oliver Fiehn²; ¹Agilent Technologies, Inc., Santa Clara, CA; ²West Coast Metabolomics Center, University of California, DAVIS, CA
- ThP 520 **Illuminating the Cellular and Molecular Response to Drug Treatment by Combining Bioenergetic Measurements with Untargeted Metabolomics**; Mark Sartain¹; Genevieve C. Van De Bittner¹; Natalia Romero²; Yoonseok Kam²; Maria Apostolidi¹; Dustin Chang¹; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, Lexington, MA

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- ThP 521 **Flexible, Vendor-agnostic Assessment of Liquid Chromatography - Mass Spectrometry System Performance using MassQL**; Heather Winter¹; Dylan J Johnson²; Alan K Jarmusch¹; ¹*Metabolomics Core Facility, Immunity, Inflammation, and Disease Laboratory, Division of Intramural Research, National Institute of Environmental Health Sciences, National Institutes of Health, Durham, North Carolina*; ²*Integrative Bioinformatics Support Group, National Institute of Environmental Health Sciences, National Institutes of Health, Durham, North Carolina*
- ThP 522 **Artificial Intelligence (AI)-Powered Discovery in Large-Scale Non-Targeted Mass Spectrometry**; Saumya Tiwari¹; Jeramie D. Watrous¹; Tao Long¹; Lori Glenwinkel¹; Igor Segota¹; Phil Worboys¹; Khoi Dao¹; Edmondo Porcu¹; Andrew Leverenz¹; Tanya Nguyen¹; Kim Lagerborg¹; Vinay Bhupathy¹; Sean Ramsey¹; Mohit Jain¹; ¹*Sapient Bioanalytics, San Diego, CA*
- ThP 523 **Microfluidic Sample-to-Analysis Platform Enables Dynamic Monitoring of Metabolic Pathways of T-Cell Activation by ESI-MS**; Austin L Culberson^{1,2}; Gianna A Slusher^{1,2,3}; Annie C Bowles-Welch⁴; Bryan Wang^{2,4,5,6}; Peter A Kottke¹; Angela C Jimenez^{2,4,5}; Krishnendu Roy^{2,4,5}; Andrei G Fedorov^{1,2,3}; ¹*The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia*; ²*National Science Foundation Engineering Research Center (ERC) for Cell Manufacturing Technologies (CMA-T), Atlanta, Georgia*; ³*Parker H. Petit Institute for Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, Georgia*; ⁴*Marcus Center for Therapeutic Cell Characterization and Manufacturing, Parker H. Petit Institute for Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, Georgia*; ⁵*The Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology and Emory University, Atlanta, Georgia*; ⁶*School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia*
- ThP 524 **A Quantitative Assay for Measuring 1000 Metabolites in Plasma Samples**; Lun Zhang¹; Jiamin Zheng¹; Mathew Johnson¹; Rupasri Mandal¹; David S. Wishart¹; ¹*University of Alberta, Edmonton, AB*
- ThP 525 **Metabolomics-Based Elucidation of Streptococcus pneumoniae and its Response to Exposure with Burkholderia-derived Alkaloids**; Mckinley D Williams¹; James L Smith^{1,2}; Thomas D Horvath³; Melinda A Engevik³; Ravi S Orugunt²; ¹*Texas A&M University, College Station, TX*; ²*Sano Chemicals, Bryan, TX*; ³*Texas Children's Hospital - Microbiome Center, Houston, TX*
- ThP 526 **Using internal standards to harmonize untargeted metabolomics data: lessons from an inter-laboratory ring trial**; Charles R Evans¹; Emily Phillips²; Yuqian Gao³; David A Gaul^{2,4}; Franklin E Leach III⁵; Brianna Garcia⁶; Kevin Cho⁷; Bradley Evans⁸; Tong Shen⁹; Shuzhao Li¹⁰; Timothy J. Garrett¹¹; Gary J. Patti¹²; Arthur Edison⁶; Xiuxia Du¹³; Facundo Fernandez^{2,4}; Oliver Fiehn⁹; Thomas O. Metz¹⁴; ¹*U of Michigan, Ann Arbor, MI*; ²*Georgia Institute of Technology, Atlanta, GA*; ³*Pacific Northwest National Lab, Richland, WA*; ⁴*Petit Institute for Bioengineering and Bioscience, Atlanta, GA*; ⁵*University of Georgia, Department of Chemistry, Athens, GA*; ⁶*University of Georgia, Athens, GA*; ⁷*Washington University in St. Louis, St. Louis, MO*; ⁸*Donald Danforth Plant Science Center, Saint Louis, MO*; ⁹*University of California Davis, Davis, CA*; ¹⁰*Jackson Laboratory, Farmington, CT*; ¹¹*University of Florida, Gainesville, Florida*; ¹²*Washington University in Saint Louis, Saint Louis, MO*; ¹³*University of North Carolina at Charlotte, Charlotte, NC*; ¹⁴*Pacific Northwest National Laboratory, Richland, WA*
- ThP 527 **Investigation of the Anti-inflammatory Effect of Astragalus radix on Mast cells using UHPLC-QTOF/MS-based Metabolomic Profiling and Pathway Analysis**; Akshay S Patil¹; Yan Xu²; ¹*Cleveland State university, CLEVELAND, OH*; ²*Cleveland State University, Cleveland, OH*
- ThP 528 **Metabolomic analysis of Rhizopus microsporus IOC4686 fungus isolated from mining environment: Screening for protein biomarkers induced by copper**; Meriellen Dias¹; Silas De Almeida Perdigão Cota De Almeida¹; Enrique Eduardo Rozas Sanchez¹; Claudio Oller Do Nascimento¹; Ricardo Pinheiro de Souza Oliveira²; Maria Anita Mendes¹; ¹*Dempster MS Lab- Poli-USP, Sao Paulo, Brazil*; ²*Faculdade de Ciências Farmacêuticas - USP, São Paulo, Brazil*
- ThP 529 **An LC-MS-based high throughput confirmative analysis of Glucose Transporter 1 (GLUT1) in human brain microvascular endothelial cells (BMECs)**; Yash Mehta¹; Dhavalkumar Patel¹; Iqra Pervaiz¹; Abraham Al-Ahmad¹; ¹*Texas Tech University Health Sciences Center, Amarillo, TX*
- ThP 530 **UPLC-ESI-MS/MS Method for the Quantitative Measurement of β -Methylamino-L-alanine in Biological Matrices**; Jenny Kim¹; Brett Bowman¹; Deepak Bhandari¹; Benjamin Blount¹; ¹*Centers for Disease Control and Prevention, Chamblee, GA*
- ThP 531 **Quantitative histone proteoform analysis of the Mus Musculus brain throughout lifespan and with life extension, spatial, and cell type specificity**; Bethany C. Taylor¹; Karl F. Poncha¹; Nicolas L. Young¹; ¹*Verna & Marrs McLean Department of Biochemistry & Molecular Biology, Baylor College of Medicine, Houston, TX*
- ThP 532 **Preliminary analyses from a planned cohort of 1,000 individuals: Cerebrospinal fluid proteomics from a multi-omic study of Alzheimer's disease**; Alexander W. Rookyard¹; Jayanta K. Chakrabarty¹; Anu Jain¹; Badri N. Vardarajan²; Min Suk Kang²; Lipi Das¹; Emily G. Werth¹; Marielba Zerlin-Esteves³; Lawrence S. Honig^{2,3,4}; Lewis M. Brown¹; Richard Mayeux^{2,3,4}; ¹*Department of Biological Sciences, Quantitative Proteomics and Metabolomics Center, Columbia University, New York, NY*; ²*Taub Institute for Research on Alzheimer's Disease and the Aging Brain, Columbia University, New York, NY*; ³*G.H. Sergievsky Center, Vagelos College of Physicians and Surgeons, Columbia University, New York, NY*; ⁴*Department of Neurology, Columbia University, New York, NY*
- ThP 533 **LC-MS/MS analysis reveals region-specific and age-related changes of glycosphingolipids in rat brain**; Tianqi Gao¹; Fanran Huang¹; Ashok Kumar²; Thomas Foster²; Zhongwu Guo¹; ¹*Department of Chemistry, University of Florida, Gainesville, FL*; ²*Department of Neuroscience, University of Florida, Gainesville, FL*
- ThP 534 **Customizing secretome analysis workflow in human iPSC-derived neurons**; Jiawei Ni¹; Ashley Frankenfield¹; Ling Hao¹; ¹*The George Washington University, Washington, DC*
- ThP 535 **Development of a robust UPLC-MS/MS method for the analysis of polyamines in biofluids and tissues from neurodegenerative diseases**; Michele Iannone¹; Liesbeth Vereyken¹; Farid Jahouh¹; Elien Grajchen¹; Sara Gorremans¹; Luc Ver Donck¹; Alexis Bretteville¹; Diederik Moechars¹; Rob J Vreeken^{1,2}; ¹*Janssen Pharmaceutica NV, Beerse, Belgium*; ²*Maastricht University, Maastricht, Netherlands*
- ThP 536 **Taking Charge: An integrative structural proteomics approach to characterize conformational behaviour of α -synuclein and effects of metal ion binding**; Emily J Byrd¹; Martin Wilkinson¹; Dale A. Cooper-Shepherd²; Sheena E Radford¹; Frank Sobott¹; ¹*The University of Leeds, Leeds, United Kingdom*; ²*Waters Corporation, Stamford Ave, Altrincham Road, Wilmslow, United Kingdom*
- ThP 537 **Proteomic analysis and characterization of detergent-insoluble proteome in Alzheimer's disease**; Masihuz Zaman¹; Yingxue Fu¹; Ping-Chung Chen¹; Huan Sun¹; Shu Yang¹; Zhiping Wu¹; Zhen Wang¹; Suresh Poudel¹; Xusheng Wang¹; Junmin Peng¹; ¹*St jude children research hospital, Memphis, TN*

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- ThP 538 **Brain derived peptide abundance correlations reveal molecular subtypes of sporadic Alzheimer's disease;** Deanna Plubell¹; Gennifer Merrihew¹; Jea Park¹; Chris Hsu¹; Christine C. Wu¹; Thomas J. Montine²; Michael J. MacCoss¹; ¹University of Washington, Seattle, WA; ²Stanford University, Stanford, CA
- ThP 539 **Whole Blood for Analysis of Neurodegenerative Disease Biomarkers;** Wenyue Zhao¹; Kevin P. Gillespie¹; Teerapat Rojsajakul¹; Clementina Mesaros¹; Ian Alexander Blair¹; ¹University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA
- ThP 540 **Synaptic dysfunction in Neurodegenerative diseases – the road from MS characterization to biofluid markers in clinical routine;** Ann Brinkmalm¹; Hlin Kvartsberg¹; Johanna Nilsson¹; Gunnar Brinkmalm¹; Henrik Zetterberg¹; Nicholas Ashton¹; Kaj Blennow¹; ¹University of Gothenburg, Molndal, Sweden
- ThP 541 **Proteomic analysis of apoE isoform effects in human iPSC-derived neurons using peptide-level analysis;** Justin McKetney^{1,2}; Einar K Krogsaeter²; Nevan J Krogan^{1,2}; Yadong Huang^{1,2}; Danielle L Swaney^{1,2}; ¹UCSF, San Francisco, CA; ²Gladstone Institutes, San Francisco, CA
- ThP 542 **Mass spectrometry-based metabolomics reveals methoxychlor-induced Parkinson's disease-like metabolic changes in C57BL/6 mice;** Fuyue Wang¹; Xiaoxiao Wang¹; Zongwei Cai¹; ¹State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, Hong Kong SAR, China, Hong Kong, China
- ThP 543 **DESI-MSI as a Complementary Tool for the Investigation of Biomarkers in Amyotrophic Lateral Sclerosis – A Pilot Study in Neurodegeneration;** Irma Berrueta Razo¹; Michael Eyres¹; Ping Yip²; Laura Ajram¹; Andrey Gagunashvili¹; Andrea Malaspina^{2,3}; Philippa J Hart¹; ¹Medicines Discovery Catapult, Manchester, United Kingdom; ²Queen Mary University of London, East London, United Kingdom; ³University College London, London, United Kingdom
- ThP 544 **Characterizing and cataloguing protein changes in Alzheimer's disease across three clinical stages of human post-mortem tissue;** Evgeny Kanshin¹; Mitchell Martá Ariza¹; Manon Thierry¹; Dominique F Leitner¹; Manor Askenazi²; Thomas Wisniewski¹; Eleanor Drummond³; Beatrice Ueberheide¹; ¹NYU Grossman School of Medicine, New York, NY; ²Biomedical Hosting LLC, Arlington, MA; ³University of Sydney, Sydney, Australia
- ThP 545 **Identification and quantification of amino acid isomerization-prone proteins in cell lysate: impact of structure and buffer conditions on protein aging;** Thomas A Shoff¹; Hoi Ting Wu¹; Joseph Geneux¹; Ryan R. Julian¹; ¹University of California, Riverside, Riverside, CA
- ThP 546 **Large-scale, deep plasma proteomics: An 1800 sample study of Alzheimer's disease;** Asim Siddiqui¹; Harendra Guturu¹; Matthijs De Geus²; Sudeshna Das²; Pia Kivisakk²; Serafim Batzoglou¹; Steven E Arnold²; ¹Seer, Inc., Redwood City, CA; ²Massachusetts General Hospital, Boston, MA
- ThP 547 **Proteomics method development for analysis of murine blood-brain barrier by spatially restricted in-vivo biotinylation;** Jan Scheibal¹; Liang Jin¹; Xue Wang¹; Chenqi Hu²; Yu Tian¹; Nadine Ruderisch³; ¹AbbVie Bioresearch Center, Worcester, MA; ²Takeda Pharmaceuticals, Cambridge, MA; ³AbbVie, Cambridge, MA
- ThP 548 **N1-Methyladenosine in RNA Contributes to Neurodegeneration Arising from CAG Nucleotide Repeat Expansion;** Yuxiang Sun¹; Hui Dai²; Xiaoxia Dai²; Jiekai Yin²; Yuxiang Cui²; Xiaochuan Liu²; Gwendolyn Gonzalez²; Jun Yuan²; Feng Tang²; Nan Wang³; Alexandra Perlegos⁴; Nancy Bonini⁴; William Yang⁵; Weifeng Gu²; Yinsheng Wang²; ¹University of California, Riverside, RIVERSIDE, CA; ²University of California Riverside, Riverside, CA; ³University of California - Los Angeles, Los Angeles, CA; ⁴University of Pennsylvania, Philadelphia, PA; ⁵University of California, Los Angeles, Los Angeles, CA
- ThP 549 **eIF5A hypusination, boosted by dietary spermidine, protects from premature brain aging and mitochondrial dysfunction;** Yongtian Liang¹; Chengji Piao¹; Christine B Beuschel¹; David Toppe¹; Laxmikanth Kollipara²; Boris Bogdanow³; Marta Maglione¹; Janine Lützkendorf¹; Jason Chun Kit See¹; Sheng Huang¹; Tim O F Conrad⁴; Ulrich Kintscher⁵; Frank Madeo⁶; Fan Liu³; Albert Sickmann⁷; Stephan J Sigrist¹; ¹Institute for Biology/Genetics, Freie Universität Berlin, Berlin 14195, Germany; ²NeuroCure Cluster of Excellence, Charité Universitätmedizin Berlin, Berlin 10117, Berlin, Germany; ³Leibniz-Institut für Analytische Wissenschaften - ISAS - e. V., Dortmund 44139, Germany, Dortmund, Germany; ⁴Department of Chemical Biology, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), 13125, Berlin, Germany; ⁵Institute for Mathematics and Computer Sciences, Freie Universität Berlin, Berlin 14195, Germany; ⁶Zuse Institute Berlin, Berlin 14195, Berlin, Germany; ⁷German Centre for Cardiovascular Research (DZHK), partner site Berlin, Berlin 10117, Berlin, Germany; ⁸Institute of Pharmacology, Center for Cardiovascular Research, Charité Universitätmedizin Berlin, Berlin 10115, Berlin, Germany; ⁹Institute of Molecular Biosciences, NAWI Graz, University of Graz, Graz, Austria; ¹⁰BioTechMed Graz, Graz, Austria; ¹¹Leibniz Institute for Analytical Sciences - ISAS - e. V., 44139, Dortmund, Germany
- ThP 550 **An Integrated omics and data-independent acquisition approach to characterize and validate the role of extracellular matrix molecules in neurodegeneration;** Joseph T. Nigro¹; Margaret Downs¹; Joseph Zaia¹; Thor D. Stein¹; Manveen K Sethi¹; ¹Boston University Chobanian and Avedisian School of Medicine, Boston, MA
- ThP 551 **A draft human brain proteome atlas for understanding the molecular basis of brain functions;** Qi Xiao¹; Yuting Xie²; Jinlong Gao¹; Hui Yang³; Zhengyi Yang⁴; Tianzi Jiang⁴; Ying Mao³; Yan Li⁵; Tiannan Guo⁶; ¹Westlake University, Hangzhou, China; ²Westlake University, Hangzhou, China; ³Fudan University, Shanghai, China; ⁴Institute of Automation, Chinese Academy of Sciences, Beijing, China; ⁵Shanghai Jiao Tong University, Shanghai, China; ⁶Westlake university, hangzhou, China
- ThP 552 **A Novel 3D Imaging Pipeline for Analyzing Efficacy of Compounds on Amyloid-Beta Plaque Dynamics in Pre-clinical Alzheimer's Disease Animal Models;** Gianna Ferron¹; Anthony Knesis¹; Stefan Linehan¹; Tim Ragan¹; Mike Sasner²; Katherine Stumpo³; Michael Easterling³; Mark Lim⁴; Gargey Yagnik⁴; Kenneth Rothschild⁴; ¹TissueVision, Inc., Newton, MA; ²The Jackson Laboratory, Bar Harbor, ME; ³Bruker Daltonics, Billerica, MA; ⁴AmberGen, Inc., Billerica, MA
- ThP 553 **CHARACTERISATION OF OLIGONUCLEOTIDES WITH PHOSPHODIESTER OR PHOSPHOROTHIOATE LINKER BY NEGATIVE ION ESI TANDEM MS AND IMS;** Fabien Hannauer¹; John Langley¹; Eugen Stulz¹; Andrew D. Ray²; Rachelle Black²; Stephen W. Holman³; ¹Chemistry, Faculty of Engineering and Physical Sciences, University of Southampton, Southampton, United Kingdom; ²New Modalities Parenteral Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Macclesfield, United Kingdom; ³Chemical Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Macclesfield, United Kingdom
- ThP 554 **A Workflow for Purity Determination, Intact Mass Measurement and MS/MS Sequencing of Oligonucleotide Impurities Detected in Synthetic Oligonucleotides;** Catalin E Doneanu¹; Jonathan Fox²; Christopher Knowles²; Ying Qing Yu³; ¹Waters Corporation, Milford, MA; ²Waters Corporation, Wilmslow, United Kingdom; ³Waters, Milford, MA
- ThP 555 **Time-course continuous monitoring of digestion reactions increases the coverage afforded by strand-**

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- cleavage approaches for the characterization of larger nucleic acids; Daniele Rollo¹; Thomas Kenderdine¹; Ghazaleh Yassaghi¹; Chris Bell²; Daniele Fabris^{1,2}; ¹University of Connecticut, Storrs, CT; ²RyboDynamics, Manchester, Connecticut
- ThP 556 **LC-MS/MS for Assessing DNA ADP-ribosylation**; Ting Zhao¹; Yun Xiong¹; ¹University of California, Riverside, Riverside, CA
- ThP 557 **High-resolution and sensitive LC-MS/MS method for the quantification of oligonucleotides**; Dilipkumar Reddy Kandula¹; Greg Roman¹; Lei Xiong²; ¹Sciex, Framingham, MA; ²SCIEX, Redwood city, CA
- ThP 558 **Development of DNA CUTaMS for sensitive quantification of damage-associated DNA modifications**; Terry D Kim¹; Ting-Yu Wang¹; Tsui-Fen Chou¹; Daniel R Semlow¹; ¹California Institute of Technology, Pasadena, CA
- ThP 559 **Nucleos'ID: new search engine enabling the untargeted identification of RNA post-transcriptional modifications from tandem mass spectrometry analyses of nucleosides**; Yannis Nicolas Francois¹; Clarisse Gosset-Erard^{1,2}; Jérôme Pansanel³; Antony Lechner⁴; Philippe Wolff⁴; Lauriane Kuhn⁵; Patrick Chaimbault²; ¹Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, Strasbourg, France; ²Laboratoire de Chimie et Physique-Approche Multi-échelles des Milieux Complexes (LCP-A2MC), Université de Lorraine, METZ, France; ³Université de Strasbourg, IPHC, CNRS, UMR7178, Strasbourg, France; ⁴Architecture et Réactivité de l'ARN (ARN) UPR 9002, CNRS, Université de Strasbourg, Strasbourg, France; ⁵Plateforme Protéomique Strasbourg Esplanade FR 1589, CNRS, Strasbourg, France
- ThP 560 **Improved Characterization of Heavily-Modified RNA Therapeutics via Electron-Based Fragmentation Methods**; Daniel Jacob Nesbitt¹; Trenton M. Peters-Clarke¹; Keaton L. Mertz¹; Michael S. Westphal^{2,3}; Trent J. Oman⁴; Joshua J. Coon^{1,2,3,5}; ¹Department of Chemistry, University of Wisconsin - Madison, Madison, WI; ²National Center for Quantitative Biology of Complex Systems, Madison, WI; ³Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI; ⁴Eli Lilly and Company, Indianapolis, IN; ⁵Morgridge Institute for Research, Madison, WI
- ThP 561 **Development of Micro Flow LC for RNA chemical modifications analysis using tandem mass spectrometry**; Qishan Lin¹; Thomas Begley¹; ¹University at Albany, Albany, NY
- ThP 562 **Fenton reaction conditions induce 5-methylcytidine increases to E.coli transfer RNAs**; Satenik Valesyan¹; Balasubrahmanyam Addepalli¹; Patrick Limbach¹; ¹University of Cincinnati, Cincinnati, OH
- ThP 563 **Stationary Phase Effects in Hydrophilic Interaction Liquid Chromatographic (HILIC) Separation of Oligonucleotides**; Scott Abernathy¹; Patrick A. Limbach¹; ¹University of Cincinnati, Cincinnati, OH
- ThP 564 **Universal Mass Exclusion List for Enhanced Modification Mapping of RNA during LC-MS/MS analysis**; Asif Ravhan¹; Balasubrahmanyam Addepalli²; Patrick A. Limbach²; ¹University of Cincinnati, Cincinnati, OH; ²University of Cincinnati, Cincinnati, OH
- ThP 565 **Studies on the stability and dissociation of tetramolecular RNA quadruplexes**; Anna Ploner¹; Sarah Viola Heel²; Kathrin Breuker²; ¹Institute of Organic Chemistry and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, Austria; ²Institute of Organic Chemistry and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, Austria
- ThP 566 **Oligonucleotide Characterization by Bio LC and Q-TOF**; Yulan Bian¹; David L Wong²; ¹Agilent Technologies, Singapore, Singapore; ²Agilent Technologies, Santa Clara, CA
- ThP 567 **Software enabled oligonucleotide mapping analysis of Erythropoietin mRNA**; Alexander Bunkowski¹; Waltraud Evers¹; Eckhard Belau¹; Thomas Meid¹; Lars Vorwerg¹; Stuart Pengelley¹; Yun Yang²; Guillaume Tremintin²; Detlev Suckau¹; ¹Bruker Daltonics, Bremen, Germany; ²Bruker Daltonics, San Jose, CA
- ThP 568 **Optimized CID conditions for 24-75mer oligonucleotide MS/MS characterization**; Stuart Pengelley¹; Eckhard Belau¹; Yeni Yung-Mui²; Dirk Wunderlich¹; Timo Schierling³; Julia Schneider³; Detlev Suckau¹; ¹Bruker Daltonics, Bremen, Germany; ²Bruker Daltonics, San Jose, CA; ³Axolabs GmbH, Kulmbach, Germany
- ThP 569 **Auto MSMS and targeted MSMS in-depth qualitative and quantitative analysis of oligonucleotide synthesis products and side products**; Detlev Suckau¹; Stuart Pengelley¹; Julia Schneider²; Timo Schierling²; Anjali Alving³; Eckhard Belau¹; Konrad Winkels¹; Lars Vorwerg¹; Alexander Bunkowski¹; ¹Bruker Daltonics, Bremen, Germany; ²Axolabs GmbH, Kulmbach, Germany; ³Bruker Daltonics, Billerica, MA
- ThP 570 **Comprehensive Characterization of tRNA by Ultra High Performance Liquid Chromatography High Resolution Accurate Mass Spectrometry**; Robert L Ross¹; Ryan Cowley²; Keeley Murphy³; Jennifer Sutton⁴; Min Du³; ¹Thermo Fisher Scientific, Franklin, MA; ²Thermo Fisher Scientific, Sunnyvale, CA; ³Thermo Fisher Scientific, Cambridge, MA; ⁴Thermo Fisher Scientific, San Jose, CA
- ThP 571 **Synthetic modified oligonucleotides analysis using a matrix-assisted laser desorption/ionization digital-ion-trap mass spectrometer (MALDI-DIT-MS)**; Yuko Fukuyama¹; Hideharu Shichi¹; Masaki Murase¹; Yoshihiro Yamada¹; Sadanori Sekiya¹; Shinichi Iwamoto¹; Koichi Tanaka¹; ¹SHIMADZU Corporation, Kyoto, Japan
- ThP 572 **A simple robust method for synthetic therapeutic RNA. New chemistry, new quantitation**; Kenneth Cook¹; Ulrik Mistarz²; Alexander Schwahn³; Keeley Murphy⁴; Yang Hao⁵; ¹ThermoFisher Scientific, Morpeth, United Kingdom; ²Thermo Fisher Scientific, Copenhagen, Denmark; ³Thermo Fisher Scientific, Reinach, Switzerland; ⁴Thermo Fisher Scientific, Cambridge, MA; ⁵Thermo Fisher Scientific, San Jose, CA
- ThP 573 **Sequence determination of long therapeutic DNA combining restriction enzyme cleavage and mass spectrometry**; Christian Sattler¹; Aref Shahnazari¹; Shima Marandi¹; Andela Juric¹; Luisa Hoffmann¹; Burak Ceylan¹; Michael Ruehl¹; ¹BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany
- ThP 574 **Validation of HILIC-HRMS Method for Quantitative Oligonucleotide Analysis**; Md Rabiul Islam¹; A M Abdullah¹; Cynthia Sommers¹; Jason Rodriguez¹; Deyi Zhang²; Darby Kozak²; Kui Yang¹; ¹Division of Complex Drug Analysis, Office of Testing and Research, Office of Pharmaceutical Quality, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Saint Louis, MO; ²Division of Therapeutic Performance I, Office of Research and Standards, Office of Generic Drugs, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Silver Spring, MD
- ThP 575 **5' mRNA Analysis By Microchip CE-MS Using an Internal Cleavage Motif for RNase H Digestion**; Adi M Kulkarni¹; Robert L Ross²; Min Du²; Kate Yu¹; ¹908 Devices, Boston, MA; ²Thermo Fisher Scientific, Cambridge, MA
- ThP 576 **Oligo Purity Analysis and Sequence Confirmation by LC/MS without Ion Pairing Reagents - Sample to reports in about 5 minutes**; Guannan Li¹; Peter Rye²; Vaughn Miller²; ¹Agilent Technologies, Santa Clara, CA; ²Agilent Technologies, Lexington, MA
- ThP 577 **Raw Material Testing: Developing Methods for Quality Control of Phosphoramidites used in the Chemical Synthesis of Oligonucleotides**; Chris Henry; Waters Corporation, Wilmslow, United Kingdom
- ThP 578 **A simple LC Orbitrap MS based poly(A) tail length assay for mRNA analysis**; Hao Yang¹; Robert Ross²;

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- Ryan Cowley³; Min Du²; ¹*Thermo Fisher Scientific, San Jose, CA*; ²*Thermo Fisher Scientific, Cambridge, MA*; ³*Thermo Fisher Scientific, Sunnyvale, CA*
- ThP 579 **Novel sample preparation platform coupled with LCMS for mRNA mass mapping**; Yun Yang¹; Guillaume Tremintin¹; Detlev Suckau²; Phillip D. Compton³; Jared J. Drader³; Sheri M Wheeler³; ¹*Bruker, San Jose, CA*; ²*Bruker Daltonics GmbH & Co.KG, Bremen, Germany*; ³*Integrated Protein Technologies Inc., Carlsbad, CA*
- ThP 580 **A Fully Automated, Sample-Specific Data Workflow for High-Throughput Identity Testing of Oligonucleotide Therapeutic**; Aude Tartiere¹; Maurizio Bronzetti¹; Stephen Kok¹; Amy Claydon²; Arnd Brandenburg³; ¹*Genedata Inc., San Francisco, CA*; ²*Genedata Ltd, Cambridge, United Kingdom*; ³*Genedata AG, Basel, Switzerland*
- ThP 581 **The advantage of LC-MS method for specific siRNA and shortmer quantitation to support mouse liver pharmacokinetics study**; Siyu Liu¹; Hefeng Zhang¹; Hongmei Wang¹; Nan Zhao¹; Zhiyu Li¹; Lili Xing¹; Yi Tao¹; Liang Shen¹; ¹*WuXi AppTec, Shanghai, China*
- ThP 582 **Rapid Structural Analysis of Peptides by Two-Dimensional Tandem Mass Spectrometry**; My Phuong Le¹; Dylan Holden¹; R. Graham Cooks¹; ¹*Purdue University, WEST LAFAYETTE, IN*
- ThP 583 **Characterizing Disulfide Bonds in Cyclic Antimicrobial Peptides with Ultraviolet Photodissociation**; Jessica Hellinger¹; Jennifer S. Brodbelt¹; ¹*University of Texas - Austin, Austin, TX*
- ThP 584 **Manual de novo sequencing of natural non-tryptic frogs' skin peptides based on EThcD method**; Irina D. Vasileva¹; Tatyana Y. Samgina¹; Albert T Lebedev^{1,2}; ¹*Lomonosov Moscow State University, Chemistry department, Moscow, Russian Federation*; ²*MASSECO doo, Postojna, Slovenia*
- ThP 585 **Merging full-spectrum and fragment ion intensity predictions from deep learning for high quality spectral libraries**; Jerry Chan¹; Henry Lam¹; ¹*Hong Kong University of Science and Technology, Hong Kong, Hong Kong*
- ThP 586 **Hydroxyproline extracted from Edmontosaurus fossil bone from the late Cretaceous**; Lucien Tuinstra¹; Brian D. Thomas¹; Steven Robinson²; Krzysztof Pawlak²; Gazmend Elezi³; Kym F. Faul³; Stephen Taylor¹; ¹*University of Liverpool, Liverpool, United Kingdom*; ²*Materials Innovation Factory, University of Liverpool, Liverpool, United Kingdom*; ³*UCLA, Los Angeles, CA*
- ThP 587 **Affinity Maturation of Macrocyclic Peptide Binders using High Throughput Screening and Automated Sequencing**; Jonathan Palmer^{1,2}; Victor Adebomi^{1,2}; Stephen Rettie^{2,3}; Jimmy Eng⁴; Gaurav Bhardwaj^{1,2,5}; Mike Guttman¹; ¹*Medicinal Chemistry, University of Washington School of Pharmacy, Seattle, WA*; ²*Institute for Protein Design, Seattle, WA*; ³*Molecular Cell and Biology program, University of Washington, Seattle, WA*; ⁴*University of Washington Proteomics Resource Center, Seattle, WA*; ⁵*Biological Physics, Structure and Design program, University of Washington, Seattle, WA*
- ThP 588 **Application of electron fragmentation strategies and software for the identification and characterization of iso-aspartate peptides in human tissue**; Blaine R Roberts¹; Ankit Jain¹; Anne M Roberts¹; Evan Hubbard²; Ryan Julian³; ¹*Emory School of Medicine, Atlanta, GA*; ²*University of California Riverside, Riverside, CA*; ³*University of California, Riverside, Riverside, CA*
- ThP 589 **Use of Ion Spectroscopy to Identify the Product Ions Created by Loss of H₂O from Protonated Polyglycine Peptides**; Allison N Fry¹; Evan Perez²; Franziska Dalhmann²; Ahmed Mohamed²; Jonathan Martens³; Giel Berden³; Theodore Corcovilos¹; Mark A. Johnson²; Michael Van Stipdonk¹; ¹*Duquesne University, Pittsburgh, PA*; ²*Yale University, New Haven, CT*; ³*FELIX Radboud University, Nijmegen, Netherlands*
- ThP 590 **Rescuing Unidentified Spectra using Self-Correcting Spectral Archival Methods in Proteomics**; Ayman Hoque¹; Long Wu¹; Henry Lam¹; ¹*Hong Kong University of Science and Technology, HONG KONG, Hong Kong*
- ThP 591 **Top-down and bottom-up proteomics on an Orbitrap Exploris 480 - Omnitrap instrument equipped with ExD, UVPD and IRMPD**; Nikita Levin^{1,2}; Athanasios Smyrnakis³; Mariangela Kosmopoulou³; Ajay Jha^{1,2}; Kyle Fort⁴; Alexander Makarov⁴; Dimitris Papanastasiou³; Shabaz Mohammed^{1,5,6}; ¹*Rosalind Franklin Institute, Harwell, Didcot, United Kingdom*; ²*Department of Pharmacology, University of Oxford, Oxford, United Kingdom*; ³*Fasmatech, NCSR Demokritos, Athens, Greece*; ⁴*Thermo Fisher Scientific, Bremen, Germany*; ⁵*Department of Biochemistry, University of Oxford, Oxford, United Kingdom*; ⁶*Department of Chemistry, University of Oxford, Oxford, United Kingdom*
- ThP 592 **Improved immunoaffinity enrichment methods for arginine methylated peptides**; Barry M. Zee¹; Hayley Peckham¹; Charles Farnsworth¹; Alissa Nelson¹; Kathryn Abell¹; Jian Min Ren¹; Michael Palazzola¹; Matthew Stokes¹; ¹*Cell Signaling Technology, Danvers, MA*
- ThP 593 **Proteome-wide direct detection and quantification of protein disulfides**; Xiaolu Li¹; Matthew Gaffrey¹; Tong Zhang¹; Song Feng¹; Wei-Jun Qian¹; ¹*Pacific Northwest National Laboratory, Richland, WA*
- ThP 594 **An improved workflow for precise and comprehensive lysine acetylole analysis**; Chia-Feng Tsai¹; Fengchao Yu²; Marina A Gritsenko¹; Rosalie K. Chu¹; Richard D. Smith¹; Alexey Nesvizhskii²; Tao Liu¹; ¹*Pacific Northwest National Laboratory, Richland, WA*; ²*University of Michigan, Ann Arbor, MI*
- ThP 595 **New Methods for fast and low cost Synthesis of stable isotope labeled (SIL) posttranslationally modified (PTM) Peptides**; Karsten Schnatbaum¹; Daniel P. Zolg²; Mathias Wilhelm³; Tobias Knaute⁴; Johannes Zerweck⁴; Holger Wenschuh⁴; Bernhard Kuster^{2,5,6}; Ulf Reimer⁴; ¹*JPT Peptide Technologies GmbH, Berlin, Germany*; ²*Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany*; ³*Computational Mass Spectrometry, Technical University of Munich, Freising, Germany*; ⁴*JPT Peptide Technologies GmbH, Berlin, Germany*; ⁵*Center for Integrated Protein Science Munich, Freising, Germany*; ⁶*Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*
- ThP 596 **Evaluating data analysis pipelines for large-scale citrullination proteomics**; Rebecca Meelker Gonzalez^{1,2}; Sophia Laposchan^{1,2}; Wassim Gabriel^{2,3}; Mathias Wilhelm^{2,3}; Chien-Yun Lee^{1,2}; ¹*Young Investigator Group: Mass Spectrometry in Systems Neurosciences, School of Life Sciences, Technical University of Munich, Freising, Germany*; ²*School of Life Sciences, Technical University of Munich, Freising, Germany*; ³*Computational Mass Spectrometry, Technical University of Munich, Freising, Germany*
- ThP 597 **Liquid Chromatography and Differential Mobility Spectrometry – Mass Spectrometry Workflow for Glycoprotein Characterization using Electron Capture and Collision Induced fragmentation**; Charlotte Jacquet¹; Gérard Hopfgartner¹; ¹*University of Geneva, Geneva 4, Switzerland*
- ThP 598 **Peptide-Spectrum Match Rescoring for Post Translational Modifications and Chemoproteomics with MSBooster and FragPipe**; Kevin L. Yang¹; Fengchao Yu²; Daniel A. Polasky²; Vadim Demichev³; Alexey I. Nesvizhskii^{1,2}; ¹*Department of Computational Medicine and Bioinformatics, Ann Arbor, MI*; ²*Department of Pathology, University of Michigan, Ann Arbor, MI*; ³*Charité – Universitätsmedizin Berlin, Berlin, Germany*
- ThP 599 **Pinpointing isomerized residue location in peptides with MS3 analysis**; Hoi Ting Wu¹; Ryan R. Julian¹; ¹*University of California, Riverside, Riverside, CA*
- ThP 600 **Proteome-wide profiling of hydroxyproline with ProAlanase and trypsin in human cell line and tissue samples**; Feixuan Wu¹; Dylan Tabang²; Hannah N. Miles³; Sara Sackett⁴; William A. Ricketts^{3,5,6}; Jon Odorico⁴; Lingjun

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- Lj^{2,3}; ¹University of Wisconsin-Madison, Madison, WI; ²University of Wisconsin-Madison, Department of Chemistry, Madison, WI; ³University of Wisconsin-Madison School of Pharmacy - Madison, WI, Madison, WI;
- ThP 601 **High-throughput Peptide Mapping for analysis of post-translational modifications and sequence variants in early development of biotherapeutics;** Vesela Encheva-Yokova¹; Sina Rafiee Mahmoudreza¹; Lukas Krasny¹; Karina Bora¹; James Graham¹; ¹Lonza, London, United Kingdom
- ThP 602 **Glycosylation site mapping using highly efficient ECD in a Q-TOF;** Joseph Meeuwse¹; Mike Hare¹; Rebecca Glaskin²; Valery Voinov¹; Joseph Beckman¹; ¹e-MSion, Corvallis, OR; ²Agilent Technologies, Santa Clara, CA
- ThP 603 **Unlocking the Potential of Site-Localized PTMs: The Power of dia-PASEF and Robust Quantification Techniques;** Justin Sing^{1,2}; Aparna Srinivasan^{1,2}; Hannes Röst^{1,2,3}; ¹Department of Molecular Genetics, University of Toronto, Toronto, ON; ²Terrence Donnelly Centre for Cellular & Biomolecular Research, Toronto, Ontario; ³Department of Computer Science, University of Toronto, Toronto, Ontario
- ThP 604 **Mass spectrometric profiling of citrullination in proteome and matrisome during human pancreas maturation and type 1 diabetes;** Hung-Yu Chiang^{1,2}; Bin Wang¹; Daniel M. Tremmel³; Sara Dutton Sackett³; Jon S. Odorico³; Lingjun Li^{1,4}; ¹School of Pharmacy, University of Wisconsin-Madison, Madison, WI; ²Biophysics Program, University of Wisconsin-Madison, Madison, WI; ³Department of Surgery, Division of Transplantation, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; ⁴Department of Chemistry, University of Wisconsin-Madison, Madison, WI
- ThP 605 **Arginylome Discovery Using an Unbiased Bottom-Up Proteomic Technique;** Joanna M Gongora¹; Zongtao Lin¹; Faith M Robison¹; Xingyu Liu¹; Yixuan (axe) Xie¹; Benjamin A. Garcia¹; ¹Department of Biochemistry and Molecular Biophysics, Washington University in St. Louis, St Louis, MO
- ThP 606 **Identifying Isomerization of Aspartic Acid Residues in Neuropeptides;** Samuel Okyem¹; Elena V. Romanova²; Jonathan V. Sweedler³; ¹University of Illinois-Urbana Champaign, Urbana, IL; ²University of Illinois Urbana Champaign, Urbana, IL; ³University of Illinois Urbana-Champaign, Urbana and Champaign, IL
- ThP 607 **Nrich(s): four strategies to delve into protein N-terminome;** Seonjeong Lee^{1,2}; Cheolju Lee^{1,2}; ¹Chemical and Biological Integrative Research Center, Korea Institute of Science and Technology, Seoul, South Korea; ²Division of Bio-Medical Science and Technology, KIST School, University of Science and Technology, Seoul, South Korea
- ThP 608 **A combined gas phase separation strategy to improve ADP-ribosylome sequencing depth;** Taku Kasai¹; Shiori Kuraoka¹; Hideyuki Higashi¹; Masanori Aikawa^{1,2,3}; Sasha A. Singh¹; ¹Center for Interdisciplinary Cardiovascular Sciences, Division of Cardiovascular Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA; ²Center for Excellence in Vascular Biology, Cardiovascular Division, Brigham and Women's Hospital, Harvard Medical School, Boston, MA; ³Channing Division of Network Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA
- ThP 609 **Improved performance of phosphopeptides characterization using online capillary electrophoresis coupling with ion mobility mass spectrometry (CE-IM-**
- MS); Ling Ling¹; Fuxing Xu¹; Chuan-Fan Ding¹; Liang Wang²; Kate Yu³; ¹Ningbo University, Ningbo, China; ²908 Devices, Shanghai, China; ³908 Devices, Boston, MA
- ThP 610 **Modification Specific Modelling in PeptideProphet Improves Validation of Rare PTM Containing Peptides in Complex Samples;** David D Shteynberg¹; Alex Zelter²; Nina Isoherranen²; Michael R Hoopmann¹; Luis Mendoza¹; Jimmy Eng²; Eric W. Deutsch¹; Robert L. Moritz¹; ¹Institute for Systems Biology, Seattle, WA; ²University of Washington, Seattle, WA
- ThP 611 **Analysis of 4-hydroxynonenal modifications in cellular retinoic acid binding protein 1 by intact protein and bottom-up mass spectrometry;** Alex Zelter^{1,2}; Ellen Riddle³; King CB Yabut³; Benjamin Zercher⁴; Alice Martynova⁴; Michael J. MacCoss⁵; Matthew F Bush⁴; Nina Isoherranen⁶; ¹Department of Genome Sciences, University of Washington, Seattle, Washington; ²Department of Biochemistry, University of Washington, Seattle, WA; ³Department of Pharmaceutics, University of Washington, Seattle, Washington; ⁴Department of Chemistry, University of Washington, Seattle, WA; ⁵Department of Genome Sciences, University of Washington, Seattle, WA; ⁶Professor and Chair, Seattle, WA
- ThP 612 **Integrating Capillary Electrophoresis and Ultraviolet Photodissociation for the Characterization of Phosphorylation States in the Carboxy-Terminal Domain of RNA Polymerase II;** Kyle Juetten¹; Jennifer Brodbelt¹; ¹University of Texas at Austin, Austin, TX
- ThP 613 **Combining Multi-Enzymatic Limited Digestion and tryptic digestion with Interpretable Machine Learning for identification and selection of PTMs-modified biomarker candidates;** Raphaël La Rocca¹; France Baumans¹; Christopher Kune¹; Jean-Luc Balligand²; Maximilien Fléron³; Dominique Baiwir³; Gauthier Eppe¹; Gabriel Mazzucchelli^{1,3}; ¹Laboratory of Mass Spectrometry, MolSys Research Unit, University of Liège, Liège, Belgium; ²Pole of Pharmacology and Therapeutics (FATH), Institut de Recherche Expérimentale et Clinique (IREC) and Department of Medicine, Cliniques Universitaires Saint-Luc, Université Catholique de Louvain, Brussels, Belgium; ³GIGA Proteomics Facility, University of Liège, Liège, Belgium
- ThP 614 **Direct determination of tyrosine sulfation sites in proteomic analysis;** Menatallah M. Yousef^{1,2}; Carson W. Szot¹; Miriam F. Ayad²; Lobna A. Hussein²; Maha F. Abdel-Ghany²; Kristina Hakansson¹; ¹University of Michigan, Ann Arbor, MI; ²Faculty of Pharmacy, Ain Shams University, Cairo, Egypt
- ThP 615 **Evaluation of MS2 Versus MS3 TMT Quantitation for Phosphotyrosine, Acetyllysine, and Methylarginine Peptides;** Alissa J. Nelson¹; Jian Min Ren¹; Anthony Possemato¹; Vicky Yang¹; Matthew Stokes¹; ¹CELL SIGNALING TECHNOLOGY, DANVERS, MA
- ThP 616 **Combination of the unique functions from timsTOF and ZenoTOF enables in-depth analysis of the glycoproteome;** Chi-Hung Lin¹; Mark Marispini¹; Wan-Fang Chou¹; Yi (jimmy) Zeng¹; Philip Ma¹; Bruce Wilcox¹; ¹PrognomiQ Inc, San Mateo, CA
- ThP 617 **FAIMS-LC/MS Reveals Structural Heterogeneity of Isoleuglandin-adducted Peptide Autoantigens;** Daniel Roeth¹; Nathaniel Bloodworth²; Wei Chen²; David M Patrick²; David G Harrison²; Markus Kalkum¹; ¹City of Hope, Duarte, CA; ²Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University Medical Center, Nashville, TN
- ThP 618 **Utilization of electron activated dissociation (EAD) on a new QTOF platform for comprehensive analysis of histone post-translational modifications;** Emily Zahn¹; Richard M Searfoss¹; Yixuan (axe) Xie¹; Zongtao Lin¹; Francisca N De Luna Vitorino¹; Benjamin A. Garcia¹; ¹Washington University School of Medicine, St. Louis, MO
- ThP 619 **Discovery of nitrotyrosine-containing proteins and peptides by antibody-based enrichment strategies;**

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- ThP 620 **Firdous Bhat¹; Kiran K. Mangalaparthy¹; Joel-Sean Hsu¹; Jane A. Peterson²; Husheng Ding¹; Dong Gi Mun¹; Akhilesh Pandey^{1,3}; ¹Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, Minnesota; ²Mayo Clinic, Rochester, Minnesota; ³Center for Individualized Medicine, Mayo Clinic, Rochester, Minnesota**
- ThP 621 **PASEF-DDA and one pot preparation of proteins for enrichment-free detection and quantitation of protein termini from pathogenic Mycobacteria; Daniel D Hu¹; Owen A Collars¹; Patricia A Champion¹; Matthew M Champion¹; ¹University of Notre Dame, Notre Dame, IN**
- ThP 622 **Rapid Automated Reaction Screening and Optimization by the Unchained Labs Junior Interfaced with Open Port Interface Mass Spectrometry; David Calabrese¹; Nate Hoxie¹; Pranav Bende¹; Meghav Verma¹; Cullen Klein¹; John Janiszewski¹; Alex Godfrey¹; Sam Michael¹; Chang Liu²; Thomas R. Covey²; ¹NIH/NCATS, Rockville, MD; ²SCIEX, Concord, ON**
- ThP 623 **A Comparative Analysis of LC-MS Based Workflows for Host Cell Protein Analysis in Bioprocess Development; Sachini P Karunaratne^{1,2}; Roger Liu¹; Chris Chumsae¹; Julia Ding¹; ¹Bristol Myers Squibb, Devens, MA; ²University of Kansas, Lawrence, KS**
- ThP 624 **Combining intact glycoprofiling and cell culture media analytics for in-process monitoring of an automated high-throughput multi-parallel bioreactor system; Yun Alelyunas¹; Charles Prochaska²; Clint Kukla²; Guillaume Bechade³; Patrick Boyce³; Mark Wrona¹; ¹Waters Corporation, Milford, MA; ²Sartorius Stedim NA, Bohemia, NY; ³Waters Corporation, Wilmslow, United Kingdom**
- ThP 625 **Automating sub-unit mAb attribute screening for in-process monitoring of an automated high-throughput multi-parallel bioreactor; Nick Pittman¹; Patrick Boyce¹; Caitlin Hanna²; Samantha Ippoliti²; Yun W Alelyunas²; Charles Prochaska³; Clint Kukla³; Guillaume Bechade¹; Magnus Wetterhall¹; Mark Wrona²; Stephan M Koza²; Ying Qing Yu²; ¹Waters Corporation, Wilmslow, United Kingdom; ²Waters Corporation, Milford, MA; ³Sartorius Stedim NA, Bohemia, NY**
- ThP 626 **Amino Acid Quantitation in Over 50 Mammalian Cell Culture Media with an Integrated CE-MS Analyzer; Kenion H Blakeman¹; Reagan Draper¹; Zhanna Sheyner¹; Ji Young Anderson¹; Scott Miller¹; ¹908 Devices, Inc., Boston, MA**
- ThP 627 **A Mass Spectrometry-Based Correlation Profiling Method for Investigating Disease Associated Alterations in Membrane Lipid-Protein Interactomes; Liuyu Peng¹; Richard G Lee²; Nichollas E Scott¹; Aleksandra Filipovska²; Gavin E Reid¹; ¹University of Melbourne, Melbourne, Australia; ²Telethon Kids Institute, Nedlands, Australia**
- ThP 628 **Parallel evaluation of ten biotin ligases for proximity proteomics; William Hardy¹; Rawan Kalloush¹; Saya Sedighi^{1,2}; Julia Kitaygorodsky^{1,2}; Vesal Kasmaeifar^{1,2}; Queenie Hu¹; Reuben Samson^{1,2}; Brendon Seale¹; Zhen-Yuan Lin¹; Cassandra Wong¹; Alexey Nesvizhskii^{3,4}; Anne-Claude Gingras^{1,2}; ¹Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto, ON; ²Department of Molecular Genetics, University of Toronto, Toronto, ON; ³Department of Pathology, University of Michigan, Ann Arbor, MI; ⁴Department of Computational Medicine and Bioinformatics, Ann Arbor, MI**
- ThP 629 **Complete structural characterization of patient-derived monoclonal autoantibodies associated with vaccine-induced thrombotic thrombocytopenia reveals the molecular mechanism of this pathology; Daniil G Ivanov¹; Son N Nguyen¹; Si-Hung Le¹; Yi Du¹; Nikola Ivetic²; Ishac Nazy²; Igor A Kaltashov¹; ¹University of Massachusetts Amherst, Amherst, MA; ²Michael G. DeGroot School of Medicine, McMaster University, Hamilton, ON**
- ThP 630 **Rapid profiling the glycosylation effects on cellular entry of SARS-CoV-2 using MALDI-MS with high mass detection; Yuye Zhou^{1,2}; Congrui Tan¹; Na Wu¹; Renato Zenobi¹; ¹ETHZ, Zürich, Switzerland; ²KTH Royal Institute of Technology, Stockholm, Sweden**
- ThP 631 **Native Mass Spectrometry for Determining the Effectiveness of Molecular Glues in Enhancing E3 Ligase-Protein Interactions for Targeted Protein Degradation; Xiaojing Huang¹; William A. Donald¹; ¹UNSW, Sydney, Australia**
- ThP 632 **Improve sensitivity, mass resolution and accuracy in micro-SEC-MS characterization of antibody-siRNA complexes; Jason X. Tang¹; Zhongping Liao¹; ¹Eli Lilly & Company, Indianapolis, IN**
- ThP 633 **Matrix-Assisted Laser Desorption/Ionization (MALDI) Studies for SARS-CoV-2 Drug Development; Congrui Tan¹; Yuye Zhou^{1,2}; Renato Zenobi¹; ¹ETH Zurich, Zurich, Switzerland; ²KTH Royal Institute of Technology, Stockholm, Sweden**
- ThP 634 **Characterization of a Nucleotide-Binding Site at the C-Terminal Domain of Human TRAP1 by Native Mass Spectrometry and Ultraviolet Photodissociation (UVPD); Hanlin Ren¹; Shanshan Yu²; Marcus Fischer²; Jennifer S. Brodbelt¹; ¹University of Texas at Austin, Austin, TX; ²St. Jude Children's Research Hospital, Memphis, TN**
- ThP 635 **Quantitative Shotgun Glycomics using Concentration-Independent (COIN) Native Mass Spectrometry; Duong T. Bui¹; James Favell¹; Elena N. Kitova¹; Zhixiong Li¹; Kelli A. McCord¹; Edward N. Schmidt¹; Fahima Mozaneh¹; Matthew S. Macauley¹; Lara K. Mahal¹; Morris R. Flynn¹; John S. Klassen¹; ¹University of Alberta, Edmonton, AB**
- ThP 636 **Membrane Proteins Enrich Distinct Lipids from Natural Lipid Extracts; Yun Zhu¹; Melanie Odenkirk²; Pei Qiao³; Jack P. Ryan⁴; Tianqi Zhang¹; Samantha Schrecke¹; Ming Zhou⁵; Mike Marty²; Erin Baker⁴; Arthur Laganowsky¹; ¹Texas A&M University, College Station, TX; ²University of Arizona, Tucson, AZ; ³Zhejiang University of Technology, Hangzhou, China; ⁴University of North Carolina at Chapel Hill, Chapel Hill, NC; ⁵Baylor College of Medicine, Houston, Texas**
- ThP 637 **Accurate golden standards and statistical models for co-fractionation mass spectrometry-based protein complex discovery; Youngwoo Lee¹; Pengcheng Yang¹; Jun Xie¹; Daniel Szymanski¹; ¹Purdue University, WEST LAFAYETTE, IN**
- ThP 638 **Insights Into the Structure and Function of Polyglutamine Disease Target DNAJB6 Using Native Mass Spectrometry; Devin M. Makey¹; Oleta T. Johnson²; Laura I. Penabad¹; Jason E. Gestwicki²; Robert T. Kennedy¹; Brandon T. Ruotolo¹; ¹University of Michigan, Ann Arbor, MI; ²University of California San Francisco, San Francisco, CA**
- ThP 639 **Automated High-throughput Online Native MS Screening for Proteins and Protein Complexes; Scott Kronewitter¹; Olufemi Adeyemi²; Paul Gazis³; Ping Yip⁴; Weijing Liu³; Albert Konijnenberg²; Rosa Viner³; Mick Greer⁵; ¹ThermoFisher Scientific, Cambridge, Massachusetts; ²ThermoFisher Scientific, Eindhoven, Netherlands; ³ThermoFisher Scientific, San Jose, CA; ⁴Thermo Fisher Scientific, Boston, MA; ⁵Thermo Fisher Scientific, Austin, TX**
- ThP 640 **Quantifying Interactions of Methylglucose Lipopolysaccharides (MGLP) with Fatty Acids Ligands; Elena Kitova¹; Duong T. Bui¹; Anna E. Grzegorzewicz²; Mary Jackson²; John S Klassen¹; ¹University of Alberta, Edmonton, AB; ²Colorado State University, Fort Collins, CO**
- ThP 641 **Online Coupling of Asymmetrical Flow Field-Flow Fractionation with Native Mass Spectrometry for Bio-Macromolecule Analysis; Tao Xing¹; Yuetian Yan¹; Shunhai Wang¹; Ning Li¹; ¹Regeneron Pharmaceuticals Inc., Tarrytown, NY**
- ThP 642 **Assembly studies of a bacterial F1FO - ATP synthase using native mass spectrometry; Alicia Just¹; Khanh Vu Huu¹; Nina Morgner¹; ¹Goethe-University, Institute of**

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- ThP 642 **Comprehensive Proteomic Interrogation of the SHOC2-MRAS-PP1C Complex;** Robert A. D'ippolito¹; Matthew Drew¹; Kelly Snead¹; Dominic Esposito¹; Frank McCormick^{1,2}; Dwight V. Nissley¹; Caroline Dehart¹; ¹Frederick National Laboratory for Cancer Research, Frederick, MD; ²Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA
- ThP 643 **Native mass spectrometry uncovers the role of Ca²⁺ and lipid binding on synaptotagmin 1 oligomerisation and function;** Sophie A. S. Lawrence^{1,2}; Tarick J. El-Baba^{1,2}; Jack L. Bennett^{1,2}; Corinne A. Lutomski^{1,2}; Carol V. Robinson^{1,2}; ¹Kavli Institute for Nanoscience Discovery, Oxford, United Kingdom; ²Department of Chemistry, University of Oxford, Oxford, United Kingdom
- ThP 644 **Structure and DNA binding of single-strand annealing proteins by native MS;** Zihao Qi^{1,2}; Charles E. Bell^{1,3}; Vicki H. Wysocki^{1,2}; ¹Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; ²Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; ³Department of Biological Chemistry and Pharmacology, Columbus, OH
- ThP 645 **Mass spectrometric analysis of acoustically activated microdroplet mediated lipid-protein complex formation;** Cheyenne P Sircher¹; Ashton Taylor¹; Theresa Evans-Nguyen¹; ¹University of South Florida, Tampa, FL
- ThP 646 **Quantifying protein co-assembly using Native Mass Spectrometry;** Wiktoria Sadowska¹; Justin Benesch¹; Dominik Saman¹; ¹Department of Chemistry, University of Oxford, Oxford, United Kingdom
- ThP 647 **A microscale proximity-dependent biotinylation procedure for low cell input samples using protease-resistant streptavidin on a magnetic substrate;** Brendon Seale¹; Reuben Samson^{1,2}; Isak Gerber³; Cassandra Wong¹; Anne-Claude Gingras^{1,2}; ¹Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Sinai Health, Toronto, ON; ²University of Toronto, Toronto, ON; ³ReSyn BioSciences, Pretoria, South Africa
- ThP 648 **Measuring the Energetics of Lipid Binding to Specific Sites on Membrane Proteins with Native MS and Mutant Cycles;** Hiruni S. Jayasekera¹; Megan Ewbank¹; Michael Thomas Marty¹; ¹University of Arizona, Tucson, AZ
- ThP 649 **Building a contaminant repository for proximity proteomics;** Julia Kitaygorodsky^{1,2}; Vesal Kasmaeifar^{1,2}; Geoffrey Hesketh³; Ugo Dionne¹; Reuben Samson^{1,2}; William Hardy¹; Rawan Kalloush¹; Saya Sedighi^{1,2}; Queenie Hu¹; Brendon Seale¹; Zhen-Yuan Lin¹; Cassandra Wong¹; Alexey I. Nesvizhskii⁴; Anne-Claude Gingras^{1,2}; ¹Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Sinai Health, Toronto, ON; ²Department of Molecular Genetics, University of Toronto, Toronto, ON; ³Department of Biochemistry and Molecular Biology, Dalhousie University, Halifax, NS; ⁴Department of Pathology, University of Michigan, Ann Arbor, MI
- ThP 650 **Proximity labeling – mass spectrometry as a tool to define DDX3X interactomes and R-loop regulators;** Thomas Beer¹; Hui Shen²; Michael C. Owens²; Qingqing Yan¹; Phillip Wulfridge¹; Kavitha Sarma¹; Kathy Fange Liu²; Hsin-Yao Tang¹; ¹The Wistar Institute, Philadelphia, PA; ²Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA
- ThP 651 **Quantifying Binding of Multiple Protein-ssDNA Homo-Oligomers Eliminates Ambiguity from Protein-Ligand Binding Measurements;** Anthony Blue¹; Alexis Edwards¹; Elyssia S. Gallagher¹; Michael A. Trakselis¹; ¹Baylor University, Waco, TX
- ThP 652 **Integrated Probabilistic Scoring of Protein-Protein Proximity Data Illuminates the Function of Dark Kinases;** Isaac B. Plutzer¹; Dhaval P. Bhatt¹; Emily M. Wilkerson¹; Dennis Goldfarb¹; M. Ben Major¹; ¹Washington University School of Medicine, St. Louis, MO
- ThP 653 **Application of Crosslinking-based technology in Quantitative Analysis of PHD2 Interactome;** Haiping Ouyang¹; Xinyu (cindy) How¹; Xiaorong (sherry) Wang²; Yao Gong¹; Lan Huang²; Yue Chen¹; ¹University of Minnesota, Minneapolis, MN; ²University of California Irvine, Irvine, CA
- ThP 654 **Native mass spectrometry unveils the details behind the GroEL allosteric functioning mechanism;** He M Sun¹; Thomas Walker¹; Arthur Laganowsky¹; Hays Rye¹; David H. Russell¹; ¹Texas A&M University, College Station, TX
- ThP 655 **Characterization of ligand – bound protein complexes using collisional-induced dissociation in tandem trapped ion mobility spectrometry/mass spectrometry (tandem-TIMS/MS);** Olufemi Samuel Araoyinbo¹; Fanny C Liu¹; Christian Bleiholder¹; ¹Florida State University, Tallahassee, FL
- ThP 656 **Coupling auxin-inducible degradation with quantitative phosphoproteomics reveals a new role for PP2ARt1 in stabilizing eisosomes during mitosis.;** Andrew Demarco¹; Mark C. Hall²; ¹Purdue University, Lafayette, IN; ²Purdue University, WEST LAFAYETTE, IN
- ThP 657 **Strategies for Deep Proteomics of Limited Tissues to Study Spatial Differentiation of Embryonic cells during Craniofacial Development;** Leena R. Pade¹; Jaeho Yoon²; Ira Daar²; Peter Nemes¹; ¹University of Maryland, College Park, College Park, MD; ²Cancer & Developmental Biology Laboratory, National Cancer Institute, NIH, Frederick, MD
- ThP 658 **Improving Proteomics Depth with nanoLC-DIMS-TIMS-MS/MS;** Cameron D. Worthington¹; Gary L. Glish¹; ¹University of North Carolina at Chapel Hill, Chapel Hill, North Carolina
- ThP 659 **Host cell proteins risk mitigation by combining 2D gel and LC-MS proteomics approaches;** Shannon Rivera¹; Chunyan Li¹; Rosalind Ang¹; Fengqiang Wang¹; Hongxia Wang¹; Hillary A. Schuessler¹; ¹Merck & Co., Inc., Kenilworth, New Jersey
- ThP 660 **Exploring the potential of negative ion mode proteomics: an MS/MS-free approach using minute time scale analysis;** Pelayo Alvarez Penanes¹; Vladimir Gorshkov¹; Mark V Ivanov²; Mikhail V Gorshkov²; Frank Kjeldsen¹; ¹University of Southern Denmark, Odense, Denmark; ²Russian Academy of Sciences, Moscow, Russia
- ThP 661 **Rapid identification of human alloantibody binding structure to human leukocyte antigen allele HLA-A*11 by cross-linking mass spectrometry;** Zheng Ser¹; Yue Gu²; Jiawei Yap²; Yanting Lim¹; Shi Mei Wang¹; Nicholas R.J Gascoigne²; Paul A Macary²; Radoslaw M Sobota¹; ¹Institute of Molecular and Cell Biology (IMCB), Agency for Science, Technology and Research (A*STAR), Singapore, Singapore; ²Department of Microbiology and Immunology, Yong Loo Lin School of Medicine, National University of Singapore, Singapore, Singapore, Singapore
- ThP 662 **Real-Time Bottom-Up Characterization of Protein Mixtures Enabled by Online Microdroplet-Assisted Enzymatic Digestion (MAED);** Cheng-Hua Ma¹; Chih-Lin Chen¹; Cheng-Chih Hsu¹; ¹Department of Chemistry, National Taiwan University, Taipei, Taiwan
- ThP 663 **An in-depth plasma proteomics workflow powered by a Novel HRAM mass spectrometer;** Amiransoor Hakimi¹; Tabiwang N. Arrey²; Jeff Op De Beeck³; Bernard Delanghe²; Sally Webb¹; Nicolaie Eugen Damoc²; ¹Thermo Fisher Scientific, San Jose, CA; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; ³Thermo Fisher Scientific - Belgium, Ghent, Belgium
- ThP 664 **A Fast and Efficient Arginine-Specific Protease for Proteomic Applications;** Chris Hosfield¹; Jessica Wohlfahrt²; Jennifer Guergues²; Ethan Strauss¹; Michael M. Rosenblatt¹; Marjeta Urh¹; Stanley Stevens Jr.²; ¹Promega Corporation, Madison, WI; ²University of South Florida, Tampa, FL
- ThP 665 **Improving Depth of Coverage and Detection of Low-Level Host Cell Proteins in Biotherapeutic Development**

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- with **Novel Functionalized Multi-Nanoparticle Platform**; Chris Sauer¹; Elsa Gorre¹; Xianglin Zhai²; Andrew Mahan¹; Hirsh Nanda¹; Aaron S Gajadhar³; Shao-yung Chen³; ¹Janssen Research and Development, Spring House, PA; ²Protein Metric Inc., Cupertino, CA; ³Seer, Inc., Redwood City, CA
- ThP 666 **Extracellular vesicles surfaceome profiling using a DTSSP cross-linking reagent and LC-ion-mobility mass spectrometry**; Hiroyuki Katayama¹; Taketo Kato^{1,2}; Palihawadana Amungama¹; Ranran Wu¹; Yining Cai¹; Fuchung Hsiao¹; Johannes Fahrman¹; Jody Vykoukal¹; Sam Hanash¹; ¹The University of Texas, Department of Clinical Cancer Prevention, Houston, TX; ²Division of Thoracic Surgery, Nagoya University, Nagoya, Japan
- ThP 667 **New and improved data acquisition schemes enabled by new functionalities of Real-Time Library Search on Orbitrap Tribrid instruments**; Peter Mowlds¹; Jenny Ho²; William Barshop³; Sebastian Gallien⁴; Jesse Canterbury⁵; ¹Thermo Fisher Scientific, Edinburgh, United Kingdom; ²Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; ³ThermoFisher Scientific, San Jose, CA; ⁴Thermo Fisher Scientific, Courtaboeuf, France; ⁵Thermo Fisher Scientific, San Jose, CA
- ThP 668 **Mass Spectrometry-based Proteomics for Microscale sample amounts: From Cells to Tissues**; Amarjeet Flora¹; Anastasia Klenke¹; Kay Opperman¹; Bhavin Patel¹; Ryan Bomgarden¹; ¹Thermo Fisher Scientific, Rockford, IL
- ThP 669 **Development of a Universal Workflow for Mass Spec Sample Prep Using Hydrophilic Magnetic Beads**; Michael Rosenblatt¹; Zhiyang Zeng²; Clara L Frazier³; Wenhui Zhou²; Marjeta Urh⁴; ¹Promega Corp, Madison, WI; ²Promega Corporation, San Luis Obispo, CA; ³University of Wisconsin-Madison, Department of Biochemistry, Madison, WI; ⁴Promega Corporation, Madison, WI
- ThP 670 **High-throughput Plasma Proteomics with High Resolution Data Independent Acquisition Method Across Multiple Orbitrap Mass Spectrometers**; Rebecca Kiss¹; Gabriel Castro²; Purvi Tandel²; Lucy Williamson²; Khatereh Motamedchaboki²; Eltaher Elgierari²; ¹Seer Inc, Redwood City, CA; ²Seer, Inc., Redwood City, CA
- ThP 671 **Comparing SP3 and SP4 Sample Preparation Techniques with a Sodium Deoxycholate-Assisted Digestion for Proteomic Profiling of MCF7 Subcellular Fractions**; Jessica M Conforti¹; Charli S. Worth¹; Amanda M. Ziegler¹; Joseph H. Taube¹; Elyssia S. Gallagher¹; ¹Baylor University, Waco, TX
- ThP 672 **ADDVenom: mass spectrometry at the heart of the development of a more effective innovative snakebite therapy based on virus-like particles**; Fernanda Gobbi Amorim¹; Damien Redureau¹; Thomas Crasset¹; Dominique Baiwir²; Stefanie Menzies³; Nicholas R. Casewell³; Loïc Quinton¹; ¹Laboratory of Mass Spectrometry, MolSys Research Unit, University of Liège, Liège, Belgium; ²GIGA Proteomics Facility, University of Liège, Liège, Belgium; ³Centre for Snakebite Research and Interventions, Liverpool School of Tropical Medicine, Pembroke Place, United Kingdom
- ThP 673 **A novel high-throughput plasma workflow facilitating fast and robust plasma proteome profiling**; Katrin Hartinger¹; Katharina Limm¹; Zehan Hu¹; Xaver Wurzenberger¹; Sebastian H. Johansson¹; Nils A. Kulak¹; ¹PreOmics GmbH, Planegg/Martinsried, Germany
- ThP 674 **Analysis of THP-1 cell secretome after LPS stimulation: comparing a nanoparticle-based workflow with traditional methods**; Giada Marino¹; Till Kindel¹; Carleen M Kluger¹; Thomas Wild¹; Nagarjuna Nagaraj¹; Andreas Tebbe¹; Catherine Pech²; Marie Guillemot²; Åsa Ehlen²; Yannick Cogne²; Pierre Olivier Maux²; François Autelitano²; ¹Evotec München GmbH, Neuried, Germany; ²EVOTEC, Toulouse, France
- ThP 675 **Early responses of human corneal and conjunctival epithelial cells to hyperosmotic stress**; Guoting Qin¹; Yunxin Fu²; Shara Duong¹; Jennifer Copeland³; Chengzhi Cai¹; ¹University of Houston, Houston, TX; ²University of Texas Health Science Center at Houston, Houston, TX; ³VICI Valco Instruments, Houston, TX
- ThP 676 **A high throughput 96 samples-per-day (SPD) workflow to quantify more than 7500 proteins from cells and complex samples**; Jan Linnemann¹; Giada Marino¹; Felix Josef¹; Till Kindel¹; Mathieu Cyrille²; Xavier Meniche²; Florian Flenkenthaler¹; Carleen M Kluger¹; Ivan Silbern¹; Thomas Wild¹; Barbara Kracher¹; Andreas Tebbe¹; Nagarjuna Nagaraj¹; ¹Evotec München GmbH, Neuried, Germany; ²EVOTEC, Toulouse, France
- ThP 677 **Ultra-High Throughput Peptide Quantification of an Acute Phase Protein Panel Using Acoustic Ejection Mass Spectrometry (AEMS) and Peptide Enrichment**; Christie Hunter¹; Bart Van Puyvelde²; Oliver Wang³; Maxim Zhgamadze³; Qin Fu³; Esthelle Hoedt³; Maarten Dhaenens²; Jennifer E. Van Eyk³; ¹SCIEX, Redwood City, CA; ²Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium; ³Cedars-Sinai Medical Center, Los Angeles, CA
- ThP 678 **Streamlined 2-min proteolytic digestion using a broad-specificity enzyme for super-fast relative and absolute quantitative proteomics**; Helen Jiang¹; Humberto Gonczarowska-Jorge²; Ying Lao¹; Victor Spicer¹; John Wilson³; Andreas Roos^{4,5}; Rene Zahedi^{1,6,7,8}; ¹Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; ²Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund 44139, Germany, Dortmund, Germany; ³ProfiIt, LLC, Fairport, NY; ⁴Department of Neuropediatrics, Developmental Neurology and Social Pediatrics, Centre for Neuromuscular Disorders in Children, University Hospital Essen, Essen, Germany; ⁵Children's Hospital of Eastern Ontario Research Institute, University of Ottawa, Ottawa, ON; ⁶Department of Internal Medicine, University of Manitoba, Winnipeg, MB; ⁷Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; ⁸CancerCare Manitoba Research Institute, Winnipeg, MB
- ThP 679 **How sweet it is: Leveraging the nuclear envelope glycome for the automated extraction of proteins from cell nuclei**; Julia E Robbins¹; Christopher Ashwood²; Erin Broderick¹; Andrea Gutierrez¹; Daniele Canzani¹; Lindsay K Pino¹; Alexander J Federation¹; ¹Talus Bioscience, Seattle, WA; ²Department of Surgery, Beth Israel Deaconess Medical Center and Harvard Medical School, Boston, MA
- ThP 680 **Improvements in real-time dynamic single-molecule protein sequencing increase proteome coverage**; Badri Singh¹; Manjula Pandey¹; Kathren Fink Croce¹; Kenneth Skinner¹; Marla Charron¹; Haidong Huang¹; Khanh D.Q. Nguyen¹; Caixia Lv¹; Juan Felipe Beltran¹; Brian D. Reed¹; ¹Quantum-Si, San Diego, CA
- ThP 681 **Deep neuron-specific proteome profiling of AAV-mediated mice brain by two-step purification**; Xue Zhang¹; Huan Sun²; Yun Jiao²; Zhiping Wu³; Junmin Peng⁴; ¹St Jude Children's Research Hospital, Memphis, TN; ²St. Jude Children's research hospital, Memphis, TN; ³St. Jude Children Research Hospital, Memphis, TN; ⁴St. Jude Children Research Hospital, Memphis
- ThP 682 **An Optimized Methodology of High-Throughput Shotgun Immunoproteomics for Antigen Identification**; Nicholas A. Shortreed¹; Anjali J. Panicker¹; Kiran K. Mangalaparthi¹; Jun Zhong¹; Akhilesh Pandey¹; Leigh G. Griffiths¹; ¹Mayo Clinic, Rochester, MN
- ThP 683 **Increasing the depth of single shot proteomics with enhanced data acquisition and processing strategies using a new Orbitrap Tribrid MS**; David Bergen¹; Jingjing Huang¹; David Horn¹; Daniel Hermanson¹; Graeme C McAlister¹; Romain Huguet¹; Bernard Delanghe²; Vlad Zabrouskov¹; ¹Thermo Fisher Scientific, San Jose, California; ²Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- ThP 684 **A high-throughput and robust multi nanoparticle-based label-free mass spectrometry workflow for deep plasma proteomics at scale**; Veder J Garcia¹; Biao Li¹; Tianyu

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- ThP 685 **Precise Recovery, Identification and Quantitation of Low Starting Protein Quantities for Bottom-up MS Analysis in the ProTrap**; Victoria Miller¹; Jessica L. Nickerson¹; Jean-François Noel²; Sara Lahsae Little¹; Angela Giraldo²; Hugo Gagnon²; ¹Allumiqs Corporation, Halifax, NS; ²PhenoSwitch Bioscience Inc., Sherbrooke, QC
- ThP 686 **High throughput total protein sequencing via multi-protease microdroplet digestion on commercially available ESI sources**; Mathew Ellenberger¹; Anastasia Lindahl¹; ¹Geltor, Emeryville, CA
- ThP 687 **A simplified high throughput cell-based assay for increased proteomic coverage of cardiomyocytes**; Saeed Sevedmohammad; Cedars Sinai Medical Institute, Los Angeles, CA
- ThP 688 **Shredder: a new way to sequence**; Alexandre Zougman¹; John Wilson²; ¹University of Leeds, Leeds, United Kingdom; ²ProtiFi, LLC, Farmingdale, NY
- ThP 689 **Automated Container-less Cell Processing Method for Single-cell Proteomics**; Cory J Matsumoto¹; Xinhao Shao¹; Marko Bogosavljevic¹; Liang Chen¹; Yu Gao¹; ¹University of Illinois at Chicago, Chicago, IL
- ThP 690 **Development of a 3D-Printed Ionization Source for Single-Cell Analysis**; Qinlei Liu¹; Sandra Martinez-Jarquín¹; Wenjie Ge²; Renato Zenobi¹; ¹Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich, Switzerland; ²Department of Biology, ETH Zurich, Zurich, Switzerland
- ThP 691 **An Optimized Workflow for TMT Based Single Cell Proteomics**; Ruiqi Jian¹; Tiffany Trinh¹; Lihua Jiang¹; Michael Snyder¹; ¹Stanford University, Stanford, CA
- ThP 692 **Single-cell lipidomic analysis by miniature dual-LIT mass spectrometry system**; Zhiyun Cai¹; Ningxi Li¹; Simin Cheng¹; Xiaoxiao Ma¹; Zheng Ouyang¹; ¹Tsinghua University, Beijing, China
- ThP 693 **Label-free single-cell proteomics made easy**; Ximena Sanchez-Avila¹; Madisyn Johnston¹; Xiaofeng Xie¹; Thy Truong¹; Kei Webber¹; Nathaniel B. Axtell¹; Veronica Puig-Sanvicens²; Ryan T. Kelly¹; ¹Brigham Young University, Provo, UT; ²HP Inc., Corvallis, Oregon
- ThP 694 **Assessing quantitation strategies for single-cell equivalent protein amounts**; Krishnatej Nishtala^{1,2}; Adrian Neild³; Alex Demarco²; Ralf B Schittenhelm¹; ¹Monash Proteomics & Metabolomics Facility, Biomedicine Discovery Institute, Monash University, Melbourne, Australia; ²Department of Biochemistry and Molecular Biology, Biomedicine Discovery Institute, Monash University, Melbourne, Australia; ³Dept. of Mechanical and Aerospace Engineering, Monash University, Melbourne, Australia
- ThP 695 **Online solid phase microextraction-capillary zone electrophoresis-tandem mass spectrometry system for single-cell proteomics**; Jorge Colon-Rosado¹; Liangliang Sun¹; ¹Michigan State University, East Lansing, MI
- ThP 696 **Extending coverage in multiplexed single-cell proteomics**; Jingjing Huang¹; Benjamin Furtwangler²; Nil Üresin²; Graeme C McAlister¹; Wang Xiao¹; Mike Goodwin¹; Jeff Op De Beeck³; Natalie Van Landuyt³; David Bergen¹; Vlad Zabrouskov¹; Romain Huguet¹; Bo Porse²; Erwin M. Schoof⁴; ¹Thermo Fisher Scientific, San Jose, California; ²Copenhagen University, Copenhagen, Denmark; ³Thermo Fisher Scientific - Belgium, Ghent, Belgium; ⁴Technical University of Denmark, Copenhagen, Denmark
- ThP 697 **Improving single-cell proteome profiling depth using single-site proteases**; Marion Pang¹; Jeff Jones¹; Nicole Kubat¹; Ting Yu Wang¹; Baiyi Quan¹; Yanping Qiu¹; Tsui-Fen Chou¹; Michael L. Roukes¹; ¹California Institute of Technology, Pasadena, CA
- ThP 698 **Accelerated Liquid Chromatography Gradient Generation with Constant-Pressure Elution Improves Sensitivity and Throughput for Single-Cell Proteomics**; Ryan Kelly¹; Xiaofeng Xie¹; Thy Truong¹; Yiran Liang¹; Madisyn Johnston¹; Kei Webber¹; ¹Brigham Young University, Provo, UT
- ThP 699 **Investigating the Metabolomics Heterogeneity of Cancer Single-Cell Using Functional Single-Cell Selection and nLC Combined with Multinozzle Emitter Mass Spectrometry**; Cheng Kai-Wen¹; Su Pin-Rui^{1,2}; Chien Miao-Ping²; Hsu Cheng-Chih¹; ¹Department of Chemistry, National Taiwan University, Taipei City, Taiwan; ²Department of Molecular Genetics, Erasmus University Medical Center, Rotterdam, Netherlands
- ThP 700 **A Novel Design for Cheap Robust Pre-Formed Step Gradient LC System**; Siqi Huang¹; Kei Webber¹; Xiaofeng Xie¹; Thy Truong¹; Ryan Kelly¹; ¹Brigham Young University, Provo, UT
- ThP 701 **High Field Asymmetric Waveform Ion Mobility Spectrometry enhances sensitivity for single cell proteomic analyses**; Eric Bonnell¹; Jiayi Peng²; Michael Belford³; Cornelia Boeser⁴; Jean-Jacques Dunyach³; Etienne Caron⁵; Aaron Wheeler²; Pierre Thibault^{1,6}; ¹Institute of Research in Immunology and Cancer, Université de Montréal, Montreal, QC; ²Institute of Biomedical Engineering, University Of Toronto, Toronto, ON; ³Thermo Fisher Scientific, San Jose, CA; ⁴Thermo Fisher Scientific, San Jose, California; ⁵CHU Sainte Justine Research Center, Montreal, QC; ⁶Department of Chemistry, Université de Montréal, Montreal, QC
- ThP 702 **Single Cell Proteome using novel Glass-Oil-Air-Droplet chip and its application on embryo development**; Liu Zhu¹; Catherine C. L. Wong^{2,3}; ¹Department of Biochemistry and Biophysics, Peking University Health Science Center, Beijing, China; ²Peking-Tsinghua Center for Life Sciences, Beijing, China; ³Department of Medical Research Center, State Key Laboratory of Complex Severe and Rare Diseases, Peking Union Medical College Hospital, Chinese Academy of Medical Science & Peking Union Medical College, Beijing, China
- ThP 703 **Detection and Quantification of Viral Proteins in Infected Cells by Single Cell Proteomics**; Akos Vegvari¹; Soham Gupta¹; Ujjwal Neogi¹; Jimmy E Rodriguez¹; Roman A Zubarev¹; ¹Karolinska Institutet, Stockholm, Sweden
- ThP 704 **Comparison of two sampling modes for single-cell metabolomics reveals alterations in senescent cells**; Catia Marques¹; Francesca Castoldi²; Liangwen Liu³; Federico Pietrocola²; Ingela Lanekoff³; ¹Uppsala University, Uppsala, Sweden; ²Karolinska Institutet, Stockholm, Sweden; ³Uppsala University, uppsala, Sweden
- ThP 705 **Top-down proteomic analysis of amount-limited samples and single cells using ultra-narrow bore open-tubular nanoflow liquid chromatography columns**; Michal Gregus¹; Yunfan Gao¹; Somak Ray¹; Alexander R. Ivanov¹; ¹Northeastern University, Boston, MA
- ThP 706 **Seamless integration of chip-based single-cell sample preparation with high-throughput liquid chromatography and diaPASEF acquisition improves sensitivity and reproducibility**; Claudia Ctordecka¹; Anjali Seth²; Michael A. Gillette^{1,3}; Namrata D. Udeshi¹; Steven A. Carr¹; ¹Broad Institute of MIT and Harvard, Cambridge, MA; ²Cellenion SASU, Lyon, France; ³Massachusetts General Hospital, Boston, MA
- ThP 707 **Highly Streamlined Chip-DIA Strategy for Microscale Phosphoproteomics from Small Cell Population to Single Cell**; Gul Muneer¹; Sofani Tafesse Gebreyesus¹; Ciao Syuan Chen¹; Tzu Tsung Lee¹; Hsiung Lin Tu¹; Yu Ju Chen¹; ¹Institute of Chemistry, Academia Sinica, Taipei, Taiwan
- ThP 708 **Lipid signatures and inter-cellular heterogeneity of naïve and lipopolysaccharide-stimulated human microglia-like cells**; Max Alexander Mueller¹; Norman Zweig¹; Bernhard Spengler²; Maria Weinert²; Sven Heiles^{3,4}.

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- ⁵; ¹*Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, 35392 Giessen, Germany;* ²*Imperial College London, London, United Kingdom;* ³*Leibniz Institute for Analytical Sciences - ISAS - e.V., 44139 Dortmund, Germany;* ⁴*Faculty of Chemistry, University of Duisburg-Essen, 44139 Essen, Germany;* ⁵*Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Germany*
- ThP 709 **High sensitivity top-down proteomics toward single cell analysis;** Zhan Gao¹; Jake A Melby²; Kalina J Reese²; Mallory C Wilson²; Daojing Wang³; Ying Ge²; ¹*UW-MADISON, Madison, WI;* ²*UW-Madison, Madison, WI;* ³*Newomics, Berkeley, CA*
- ThP 710 **Optimization of targeted proteomics for single glomerulus measurements;** Chris Hsu¹; Lillian R. Heil¹; Philip M Remes²; Ping Yip²; Jesse D. Canterbury²; Christine C. Wu¹; Mariya T. Sweetwyne¹; Michael J. MacCoss¹; ¹*University of Washington, Seattle, WA;* ²*Thermo Fisher Scientific, San Jose, California*
- ThP 711 **Combining single-cell mass spectrometry and transferable meta-learning framework to predict cell phenotypes;** Yunpeng Lan¹; Tra D. Nguyen¹; Songyuan Yao¹; Yihan Shao¹; Zhibo Yang¹; ¹*University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK*
- ThP 712 **Improving protein quantification for single cell proteomics;** Hannah Boekweg¹; Alexander Solivais²; Daisha Van Der Watt¹; Sarah Fund¹; Ansima R Mongane¹; Michael R. Shortreed²; Sam Payne¹; ¹*Brigham Young University, Provo, UT;* ²*University of Wisconsin-Madison, Madison, WI*
- ThP 713 **Nano-LC-MS based lipidomics for Single Cell Applications;** Rahul Ravi Deshpande¹; Bashar Amer¹; Amirmansoor Hakimi¹; Jeff Op De Beeck²; Thomas Moehring²; Susan Bird¹; ¹*Thermo Fisher Scientific, San Jose, California;* ²*Thermo Fisher Scientific, Bremen, Germany*
- ThP 714 **Short and Long-term Stability of Aromatic Amines in Human Urine;** Shrila Mazumder¹; Rayaj A. Ahamed¹; Tiffany H. Seyler¹; Lanqing Wang¹; ¹*Centers for Disease Control and Prevention, Atlanta, GA*
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- ThP 716 **Sensitive quantification of the protein targeting chimera (PROTAC) TL 13-112 in rat plasma using an LC-MS/MS workflow;** Ebru Selen¹; Rahul Baghla¹; Eshani Nandita¹; ¹*SCIEX, Redwood City, CA*
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- ThP 719 **Low-level quantification of 10 mutagenic nitrosamine impurities in Pioglitazone hydrochloride using accurate mass spectrometry;** Eshani Nandita¹; Rahul Baghla¹; Lakshmanan Deenadayalan²; Jack Steed³; ¹*SCIEX, Redwood City, CA;* ²*SCIEX, Bangalore, India;* ³*SCIEX, Macclesfield, United Kingdom*
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