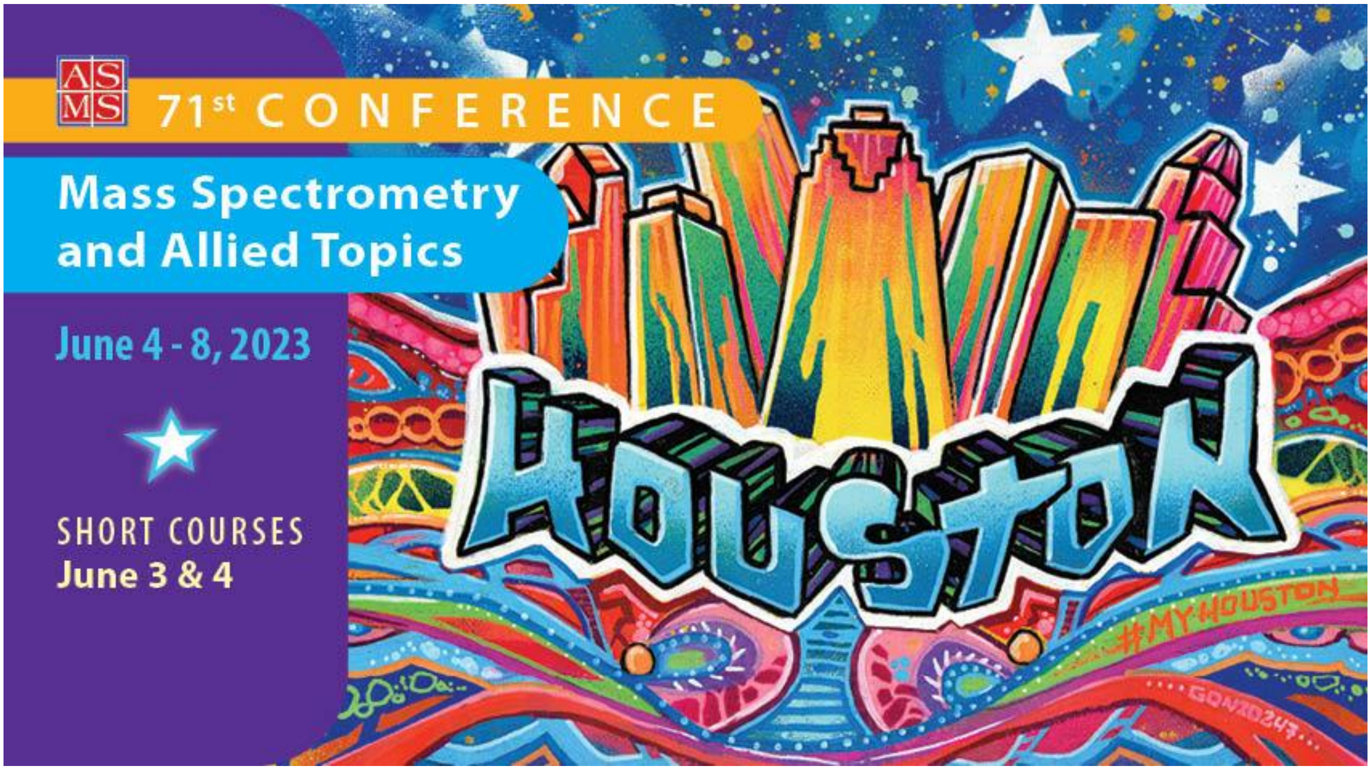

FINAL PROGRAM

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** *Baylor College of Medicine* **Tutorial Session II,** Ballroom A 5:00 – 5:45 pm **Mass Spectrometry and Anti-Doping Research** **Mario Thevis** *Institute of Biochemistry, Center for Preventive Doping Research, German Sport University Cologne*
	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**, *University of California, Los Angeles* 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** *Department of Human Biology at Maastricht University Medical Centre+*
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	**Oral Sessions** 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
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Monday Posters, Halls BC **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 11:30 am - 1:00 pm: **Undergraduate students** look for reserved tables and free lunch vouchers to ***Meet the Experts***
2:30 - 4:30 PM	**Oral Sessions** 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
4:45 - 5:30 PM	**Award Lecture,** Hall A **John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry** preceded by Al Yergey MS Scientist Award Presentations **Carol V. Robinson** *University of Oxford*
5:45 - 7:00 PM	**Workshops** There are light refreshments in foyers, 5:30 - 5:45 pm. 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 Exposome research: overcoming challenges to deliver answers, Room 360 CF 17 Using Casanovo for de novo peptide sequencing, Room 361 ABDE
7:00 - 8:00 PM	**Special Gap Hour Reception sponsored by AGILENT,** Ballroom B Reception immediately following workshop *06 Networking for Scientists: Celebrating Women Mass Spectrometrists*. All are welcome to join for networking focused on supporting women in mass spectrometry and the FeMS organization.
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	**ORAL SESSIONS** TOA am: Instrumentation: New Developments in Ionization and Sampling (In Memory of Marvin Vestal), Hall B3 TOB am: Biomarkers: Quantitative Analysis, Grand Ballroom A TOC am: Fundamentals: Native MS and Structures of Large Ions , Grand Ballroom B TOD am: Informatics: Peptide and Protein Identification, Proteomics, Grand Ballroom C TOE am: Exposomics, Toxicology, and Health Outcomes, Room 332 TOF am: Neurodegenerative Disease Research, General Assembly A TOG am: Drug Metabolism and Pharmacokinetics, General Assembly B TOH am: Imaging: Spatially-Resolved Omics, General Assembly C
10:30 AM - 2:30 PM	**POSTER SESSION AND EXHIBITS,** Tuesday Posters, Halls BC **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
2:30 - 4:30 PM	**ORAL SESSIONS** TOA pm: Instrumentation: High-Resolution Mass Spectrometry, Hall B3 TOB pm: Post-translational Modifications: Qualitative & Quantitative Analysis, Grand Ballroom A TOC pm: Fundamentals: Ionization Methods, Grand Ballroom B TOD pm: Informatics: Multiomics Integration and Applications, Grand Ballroom C TOE pm: Plants and Natural Products, Room 332 TOF pm: Ion Mobility: Structure Determination & Applications, General Assembly A TOG pm: H/D Exchange: Innovations and Applications, General Assembly B TOH pm: Clinical Analysis: Applications, General Assembly C
4:45 - 5:30 PM	**AWARD LECTURE, HALL B3** **Biemann Medal Lecture** preceded by **Research Award Presentations** **Brandon Ruotolo** *University of Michigan*
5:45 - 7:00 PM	**WORKSHOPS** There are light refreshments in foyers, 5:30 - 5:45 pm. 01 Open and Reproducible Data Analysis for FT-MS, Room 310 A 02 Accelerator Mass Spectrometry (AMS): Current Utility and Future Opportunities , Room 310 BC 03 Constructing an Individual Development Plan (IDP), Room 320 A 04 The NIH and NSF Review and Funding Process, Room 320 BC 05 From data to biology: using -omics datasets to generate an unbiased hypothesis , Ballroom A 06 Recognizing the “A” in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists, Ballroom B 07 Data Independent Acquisition: After the Acquisition, Ballroom C 08 FAIR Data Sharing Principles and Barriers: the New NIH Data Management and Sharing (DMS) Policy, Room 332 09 Kahoot Trivia! LCMS (and other topics) , General Assembly A 10 Lipidomics: What does International Lipidomics Society offer to the lipidomic community?, General Assembly B 11 Native MS: new approaches to enable discovery in academia and industry, General Assembly C 12 New fragmentation methods as seen through the lens of radical ion chemistry, Room 340 AB 13 Non-target analysis (NTA): Modern tools for unknown analysis, Room 351 ABDE 14 Trans-Proteomic Pipeline: Recent Advances and Future Directions, Room 351 CF 15 Imaging MS: Isomer Differentiation in Biological Imaging, Room 360 ABDE 16 Mass Spectrometry Support for Extractables and Leachables and Biocompatibility testing, Room 360 CF 17 Mass Spectral Tools to Enhance Characterization and Identification of Forensic Evidence, Room 361 ABDE17 Visualization of Mass Spectrometry related data (Interest Group: Bioinformatics MS), *Room 200 HI*
7:00 - 8:00 PM	**SPECIAL GAP HOUR RECEPTION SPONSORED BY SCIEX,** Ballroom B Reception immediately following workshop *06 Recognizing the “A” in DEIA: Effective Ways to Improve Accessibility for Mass Spectrometrists.* All are welcome to join for networking focused on accessibility, diversity and inclusion.
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	**Oral Sessions** 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
10:30 am - 2:30 pm	**Poster Session and Exhibits,** Wednesday Posters, Halls BC **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
2:30 - 4:30 pm	**Oral Sessions** 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
4:45 - 5:30 pm	**ASMS Meeting,** Hall B3. Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 pm	**Workshops** There are light refreshments in foyers, 5:30 - 5:45 pm. 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
7:00 - 8:00 pm	**Special Gap Hour Reception sponsored by SEER,** Ballroom B Reception immediately following workshop *06 MS Career Options: How to Kick Start Your Career*. All are welcome to join for networking focused on career development.
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	**Oral Sessions** 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
10:30 AM - 2:30 PM	**Poster Session and Exhibits,** Thursday Posters, Halls BC **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
2:30 - 4:30 PM	**Oral Sessions** 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
4:45 - 5:30 PM	**Plenary Lecture,** Hall B3 **The Rise and Reign of the Mammals: A New History, from the Shadow of the Dinosaurs to Us** **Stephen Brusatte** *University of Edinburgh*
7:00 – 10:00 PM	**Closing Event at the Houston Museum of Natural Science** **Advance purchase ticket is required**. Ticket sales CLOSE on Monday June 5, 12pm noon. 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. 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. The Houston Museum of Natural Science is located at 5555 Hermann Park Drive, Houston TX 77030. If you do not wish to take the light rail, Uber/Lyft or taxis are available.

MOA am: Top Down Protein Analysis
Hall B3
Session Chair: Frederik Lermyte (Technical University of Darmstadt)

MOA am 08:30 **Proteoforms - how can we transfer them intact from tissues into mass spectrometers?**; Hartmut Schlüter[1]; Jan Hahn[1]; Manuela Moritz[1]; Hannah Voss[1]; Marcel Kwiatkowski[2]; *[1]UKE - Section Mass Spectrometry and Proteomics, University of Hamburg, Hamburg, Germany; [2]Functional 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 Hinkle[4]; Idlir Liko[5]; Andrew Dolan[1, 2]; Christopher Mullen[6]; John E.P. Syka[6]; Carol V Robinson[1, 2]; *[1]Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; [2]University of Oxford, Oxford, United Kingdom; [3]School of Chemistry, UNSW Sydney, Sydney, Australia; [4]Thermo Fisher Scientific, San Jose, California; [5]OMass Therapeutics, Oxford, United Kingdom; [6]Thermo Fisher Scientific, San Jose, CA*

MOA am 09:10 **Native top-down mass spectrometry approaches to determine the FraB/FrlB-substrate binding sites and conformational changes induced by substrate binding**; Yuan Gao[1]; Sravya Kovvali[2]; Jamison Law[1]; Venkat Gopalan[1]; Vicki H Wysocki[1]; *[1]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; [2]The 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 Guthals[1]; Derrill Sturgeon[1]; Alexander Gavrilenko[1]; Blake Hakkila[1]; Stephanie Sturgeon[1]; Jhenya Gavrilenko[1]; Rachel Franklin[1]; Yury Vasil'ev[1]; Joseph Meeuwsen[1]; Valery Voinov[1]; Joseph Beckman[1]; *[1]e-MSion, Corvallis, OR*

MOA am 09:50 **Internal Fragment Assignment Challenges in Top-Down Electron Capture Dissociation Tandem Mass Spectrometry**; Neven N. Mikawy[1]; Carolina Rojas Ramírez[1]; Brandon T. Ruotolo[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, Michigan*

MOA am 10:10 **Unravelling proteoform footprints of proteasome subtypes using top-down mass spectrometry**; Angelique Sanchez Dafun[1]; Dusan Zivkovic[1]; Stephen Adonai Leon Icaza[1]; Sophie Moeller[2]; Carine Froment[1]; Delphine Bonnet[3, 4]; Adriana Almeida De Jesus[5]; Laurent Alric[4]; Muriel Quaranta-Nicaise[3]; Audrey Ferrand[3]; Céline Cougoule[1]; Etienne Meunier[1]; Odile Burlet-Schiltz[1]; Frédéric Ebstein[2]; Raphaela Goldbach-Mansky[5]; Elke Krüger[2]; Marie-Pierre Bousquet[1]; Julien Marcoux[6]; *[1]IPBS Toulouse, Toulouse, France; [2]Institute of Medical Biochemistry and Molecular Biology, University Medicine Greifswald, Greifswald, Germany; [3]IRSD, Université de Toulouse, INSERM, INRA, INP ENVT, Université de Toulouse 3 Paul Sabatier, Toulouse, France; [4]Internal medicine department of digestive disease, Rangueil Hospital, Université de Toulouse III - Paul Sabatier (UPS), Toulouse, France; [5]NIH/NIAID, Bethesda, MD; [6]CNRS, 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 Green[1]; Sadia Sheraz[1, 2]; Elena Castellani[1, 3]; Zoltan Takats[1, 4]; Nick Lockyer[2]; *[1]Rosalind Franklin Institute, Harwell, Didcot, United Kingdom; [2]University of Manchester, Manchester, United Kingdom; [3]University of Oxford, Dept. of Chemistry, Oxford, United Kingdom; [4]Imperial 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 Grgic[1]; Benjamin Bartels[1]; Alexandros Lekkas[2]; Diamantis Kounadis[2]; Elias Panagiotopoulos[2]; Dimitris Papanastasiou[2]; Ron M.A. Heeren[1]; Shane R. Ellis[1, 3, 4]; *[1]M4i - Maastricht MultiModal Molecular Imaging Institute, Maastricht University, Maastricht, Netherlands; [2]Fasmatech, NCSR Demokritos, Athens, Greece; [3]Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; [4]Illawarra Health and Medical Research Institute, Wollongong, Australia*

MOB am 09:10 **Multimodal IR-Guided MALDI Imaging of Biological Samples at High Spatial Resolution**; Ethan Yang[1]; Peng Wang[2]; Joshua L Fischer[1]; Thomas Tague[2]; Marten Seeba[3]; Hans-Christian Koch[3]; Tim Rider[2]; Katherine Stumpo[1]; Michael Easterling[1]; *[1]Bruker Daltonics, Billerica, MA; [2]Bruker Optics Inc, Billerica, MA; [3]Bruker 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. Weigand[1]; Daisy M. Unsihuay Vila[1]; Manxi Yang[1]; Hang Hu[1]; Shane Tichy[2]; Julia Laskin[1]; *[1]Purdue University, Dept. of Chemistry, West Lafayette, IN; [2]Agilent 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 Kanchustambham[1]; Pei Su[1]; Jared O. Kafader[1]; Neil L. Kelleher[1]; *[1]Northwestern 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 Jones[1]; Emmy Hoyes[2]; Scott Trinkle[3]; Richard Chapman[4]; *[1]Waters, Wilmslow, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters, Milford, MA; [4]Waters 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 Nartey[1]; Abanoub Mikhael[1]; Helena Petrosova[1]; Michael X Chen[2]; Robert K Ernst[3]; David R Goodlett[1]; *[1]University of Victoria, Victoria, BC; [2]UBC, Vancouver, BC; [3]University 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 Isenberg[1]; C. Austin Pickens[1]; Adrienne Manning[2]; Carla Cuthbert[1]; Konstantinos Petritis[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA; [2]Katherine A. Kelley State Public Health Laboratory, Rocky Hill, CT*

MOC am 09:10 **Rapid ICP-MS Analysis of Dried Blood Spots via Direct Microextraction from Solid Substrates**; R. Kenneth Marcus[1]; Cameron J. Stouffer[1]; [1]*Clemson University, Clemson, SC*

MOC am 09:30 **A generic loading strategy for automated sample loading of Evotips for robust and high throughput analysis on the Evosep One**; Magnus Huusfeldt[1]; Dorte B. Bekker-Jensen[1]; Jacob Poder[1]; Moritz Heusel[1]; Lasse Falkenby[1]; Nicolai Bache[1]; [1]*Evosep, Odense, Denmark*

MOC am 09:50 **On-site Breast Cancer Diagnosis Using Paper Spray Ionization Miniature Mass Spectrometry**; Cheng-Chih Hsu[1]; Hou-Chun Huang[1]; Hsin-Hsiang Chung[1]; Jia-Ying Yu[1]; Bo-Rong Chen[2]; Ming-Yang Wang[2]; [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-Navas[1]; Md Amir Hossen[2]; Mohamed Boutaghou[2]; Arif Kocabas[1]; Manuel Gonzalez[1]; Isaac Marin-Valencia[1]; [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 Nakamura[1]; Toshihiko Nogawa[1]; [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, 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 Tajaddodi[1]; Hayden Thurman[1]; Billy Kantharidis[2]; Alexandre A. Shvartsburg[1]; 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 Yao[1]; Qian Ruan[1]; [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 Wu[1]; Chuan-Fan Ding[2]; [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 Trinh[1]; Sophie Liuu[2]; Chenqin Cao[3]; Ekaterina Darii[4]; Jean-Claude Tabet[3, 5]; Annelaure Damont[3]; François Fenaille[3]; Olivier Firmesse[2]; Jacques-Antoine Hennekinne[2]; Chanthadary Inthavong[1]; Gwenaelle Lavison-Bompard[1]; [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 Hayward[1]; Allie Ferranti[1]; Thomas Wolf[2]; Jan-Christoph Wolf[2]; [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 Quinn[1]; Yunhe Hong[1]; Nicholas Birse[1]; Chris Elliott[1]; [1]*Queen's University Belfast, Belfast, United Kingdom*

MOE am 09:50 **A comparative untargeted metabolomics analysis of açaí (Euterpe oleracea Mart.) fruit, food powder, and botanical dietary supplement extracts**; Kabre L. Heck[1]; Lauren E. Fogel[1]; Yuyan Yi[2]; Jingyi Zheng[2]; Angela I. Calderon[1]; [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 Xu[1]; Hong Chen[1]; Huan Zhang[1, 2]; Michael W. Crowder[2]; Jiangjiang Zhu[1]; [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**; Keriann Backus[1]; Nikolas Burton[2]; Flowreen Shikwana[2]; Daniel Polasky[3]; Samuel Ofori[2]; Daniel Geiszler[3]; Alexey I Nesvizhskii[3]; [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. Amaral[1]; Andrew R. M. Michael[1]; Raja S. Kondrapolu[2]; Darin E. Jones[2]; David C. Schriemer[1]; [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 Sun[1]; Mierxiati Saimi[2]; Qing Cao[2]; Don L. Rempel[1]; Mengqi Chai[3]; Weikai Li[2]; Michael L. Gross[1]; *[1]Washington University in St.Louis, St.Louis, MO; [2]Washington University School of Medicine, St. Louis, MO; [3]Washington university in St louis, St Louis, MO*

MOF am 09:30 **qXL-MS elucidation of membrane protein unfolding to visualize membrane complexes dynamics**; Anna Bakhtina[1]; Sung-Gun Park[1]; Martin M. Mathay[1]; James E. Bruce[1]; *[1]University of Washington, Seattle, WA*

MOF am 09:50 **Defining the Structures and Interactions of the Human Platelet Secretome using Chemical Crosslinking**; Michelle Cielesh[1]; Jemma Fenwick[1]; Fay Ghani[1]; Yvonne Kong[1]; Freda H Passam[1]; Mark Larance[1]; *[1]Charles 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 Chea[1]; Zhi Cheng[1]; Jiana Duan[1]; Tyler Fletcher[1]; Scot Weinberger[1]; *[1]GenNext 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 Bochenek[1]; Kayla N Williams-Pavlantos[1]; Andrew S McGee[1]; Chrys Wesdemiotis[1]; *[1]The 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 Charles[1]; Thierry NJ Fouquet[2]; Jean-Arthur Amalian[3]; Isaure Sergent[4]; Pierre Giusti[5, 6]; Didier Gigmes[4]; *[1]Aix-Marseille University, Marseille Cedex 20, France; [2]Bausch+Lomb, Rochester, NY; [3]Sanofi, Aramon, France; [4]Aix Marseille Université, CNRS, Institut de Chimie Radicalaire,, MARSEILLE, France; [5]TotalEnergies OneTech R&D, TotalEnergies Research & Technology, Gonfreville, France; [6]International 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. Grayson[1]; Mckenna J. Redding[1]; Kayla N Williams-Pavlantos[2]; Oluwapelumi O. Kareem[1]; Chrys Wesdemiotis[2]; *[1]Tulane University, New Orleans, LA; [2]University of Akron, Akron, OH*

MOG am 09:30 **Characterization of Modified Hyaluronic Acid Materials and Their Interaction with Contact Lenses**; Michelle L. Piotrowski[1]; Andrew J. Hoteling[1]; *[1]Bausch+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 Arnould[1]; Aparna Annamraju[2]; Ercan Cakmak[2]; Frederic Vautard[2]; *[1]Bruker Scientific, LLC, Billerica, MA; [2]Oak Ridge National Laboratory, Oak Ridge, TN*

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 Mazzah[1]; Youssef Bakkour[2, 3]; Christian Rolando[1, 4]; *[1]Miniaturization for Synthesis, Analysis & Proteomics (MSAP), USR 3290, CNRS, University of Lille, Faculty of Sciences & Technologies, 59655 Villeneuve d'Ascq cedex, France; [2]Laboratory of Applied Chemistry (LAC), Lebanese University, Faculty of Sciences, Tripoli, Lebanon; [3]College of Applied Medical Sciences, King Khalid University, Abha, Saudi Arabia; [4]Shrieking Sixties, 1-3 Allée Lavoisier, 59650 Villenueve 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 Wang[1]; Mingxun Wang[2]; *[1]University of California, Riverside, riverside, CA; [2]University of California, Riverside, Riverside, CA*

MOH am 08:50 **An Automated Workflow Composition System In LC-MS Metabolomics Data Processing**; Xinsong Du[1]; Farhad Dastmalchi[1]; Matthew A. Diller[1]; Mathias Brochhausen[2]; Timothy J. Garrett[1]; William R. Hogan[1]; Dominick J. Lemas[1]; *[1]University of Florida, Gainesville, FL; [2]University 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 Stratton[1]; Rachel Richardson[1]; Jennifer E. Kyle[1]; Josie G. Eder[1]; Kristin M Engbrecht[1]; Athena A. Schepmoes[1]; Bobbie-Jo Webb-Robertson[1]; Lisa M Bramer[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

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

MOH am 09:50 **Development of Aggregated Molecular Phenotype (AMP) Scores to Associate and Visualize Molecular Changes**; Jessie Chappel[1]; Mary King[2]; Rachel Dehoog[2]; Livia S. Eberlin[2]; David Reif[3]; Erin S. Baker[4]; *[1]North Carolina State University, Raleigh, NC; [2]Baylor University, Waco, TX; [3]National Institute of Environmental Health and Sciences, Raleigh, North Carolina; [4]University 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 Köhler[1]; Vivian Würf[1]; Josch K Pauling[1]; *[1]LipiTUM, Technical University of Munich, Freising, Germany*

MOH pm 02:30 **Speeding up proteomics using a micro-flow LC timsTOF-HT**; Johanna Tüshaus[1]; Claire Delbridge[2]; Eike Mucha[3]; Christoph Krisp[4]; Jürgen Schlegel[2]; Bernhard Kuster[1]; *[1]Technical University of Munich, Freising, Germany; [2]Technical University of Munich, Munich, Germany; [3]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [4]Bruker 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. Rosenberger[1]; Marvin Thielert[1]; Maximilian T. Strauss[2]; Katherine Madden[1]; Constantin Ammar[1]; Sophia C. Maedler[1]; Lisa Schweizer[1]; Andreas Metousis[1]; Patricia Skowronek[1]; Maria Wahle[1]; Edwin Rodriguez[1]; Thierry M. Nordmann[1]; Andreas Mund[2]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Novo 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 Nguyen[1]; Lindsie Martin[1]; Zongkai Peng[1]; Rakhi Rajan[1]; Zhibo Yang[1]; *[1]University 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. Gomes[1]; Blandine Chazarin[2]; Aleksandra Binek[2]; Jolene K. Diedrich[1]; Jennifer E. Van Eyk[2]; John R. Yates III[1]; *[1]Scripps Research, La Jolla, CA; [2]Advanced 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 Vrsanova[1]; Syed Azmal Ali[1]; Mathias Kalxdorf[2]; Jeroen Krijgsveld[1]; *[1]German Cancer Research Center, Heidelberg, Germany; [2]Cellzome GmbH (a GSK company), Heidelberg, Germany*
MOA pm 03:50	**Electrophoresis-Correlative Mass Spectrometry Enables Ultrasensitive Proteomics**; Bowen Shen[1]; Peter Nemes[1]; *[1]University 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. Arrey[1]; Bernard Delanghe[1]; Santosh Renuse[2]; Jeff Op De Beeck[3]; Paul Jacobs[3]; Nicolaie Eugen Damoc[1]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Thermo Fisher Scientific, San Jose, California; [3]Thermo 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 Sommertune[1]; Emily R. Sekera[2]; Bela Paizs[3]; Zoltan Takats[3]; Arpad Somogyi[2]; *[1]Polymer Factory Sweden, Stockholm, Sweden; [2]The Ohio State University, Columbus, OH; [3]Rosalind 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 Habibi[1]; Gabe Nagy[1]; *[1]University 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. Huntley[1]; Adam L. Hollerbach[1]; Aneesh S. Prabhakaran[1]; Cameron M. Giberson[1]; Randolph V. Norheim[1]; Richard D. Smith[1]; Yehia M. Ibrahim[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*
MOB pm 03:30	**Leveraging High-Resolution SLIM-IMS Separations with Selective Ion-Neutral Clustering, HDX, and Cryogenic IR Spectroscopy**; Vasyl Yatsyna[1]; Brian H Clowers[2]; Thomas Rizzo[1]; *[1]Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland; [2]Washington State University Department of Chemistry, Pullman, WA*
MOB pm 03:50	**Native mass spectrometry on a modified timsTOF Pro**; Yu-Fu Lin[1]; Angela Di Capua[1]; Erin Panczyk[2]; Benjamin Jones[2]; Mark Ridgeway[2]; Arpad Somogyi[1]; Desmond Kaplan[3]; Melvin Park[2]; Vicki Wysocki[1]; *[1]The Ohio State University, Columbus, OH; [2]Bruker Daltonics, Billerica, MA; [3]KapScience 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 Lee[3]; Christopher J. Hogan[3]; Carlos Larriba-Andaluz[4]; *[1]Indiana University Purdue University - Indianapolis, Indianapolis, IN; [2]Purdue University, Lafayette, IN; [3]University of Minnesota, Minneapolis, MN; [4]Indiana 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'Reilly[1]; Andrea Graziadei[2, 3]; Christian Forbrig[2]; Rica Bremenkamp[4]; Jörg Stülke[4]; Juri Rappsilber1[2]; *[1]NCI NIH, Frederick, MD; [2]Technische Universität Berlin, Berlin, Germany; [3]Human Technopole, Milan, Italy; [4]University 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 Muehlberg[1]; Boris Bogdanow[1]; Kenta Okamoto[2]; Liu Fan[1]; *[1]Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; [2]Uppsala 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 Zhou[1]; Giovanna Scapin[1]; Yacob Gomez Llorente[1]; Terri Kelly[1]; David McLaren[1]; Songnian Lin[1]; James Mu[1]; *[1]Merck & Co., Inc., Kenilworth, New Jersey*
MOC pm 03:30	**Unravelling the Mechanism of Rotavirus Viral Factory Formation using Structural Mass Spectrometry**; Alice Colyer[1]; Julia Acker[2]; Xinyu Wang[2]; Alexander Borodavka[2]; Antonio Calabrese[1]; *[1]University of Leeds, Leeds, United Kingdom; [2]University of Cambridge, Cambridge, United Kingdom*
MOC pm 03:50	**Direct determination of membrane protein complexes from cellular membranes**; Wonhyeuk Jung[1]; Aniruddha Panda[1]; Kallol Gupta[1]; *[1]Yale 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]; Idlir Liko[5]; Joshua D Hinkle[6]; Christopher Mullen[7]; John E.P. Syka[7]; Carol V Robinson[1, 2]; *[1]Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; [2]Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom; [3]Department of Chemistry, University of Oxford, Oxford, United*

Kingdom; [4]School of Chemistry, UNSW Sydney, Sydney, Australia; [5]OMass Therapeutics, Oxford, United Kingdom; [6]ThermoFisher Scientific, San Jose, CA; [7]Thermo 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**; Maria Fernanda Cifuentes Girard[1]; Gérard Hopfgartner[1]; *[1]University 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 Michael[1]; Alan T Maccarone[1]; Todd W Mitchell[1]; Christer S Ejsing[2, 3]; Shane R. Ellis[1]; *[1]School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; [2]Department of Biochemistry and Molecular Biology, Villum Center for Bioanalytical Sciences, University of Southern Denmark, Odense, Denmark; [3]Cell 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 Abril[1]; Jeremy Koelmel[2]; Michael Kummer[1]; Ralph Hindle[3]; Kathy Hunt[3]; Stephan Baumann[4]; Krystal J Godri Pollitt[2]; Emma E Rennie[4]; *[1]Innovative Omics, Sarasota, FL; [2]Yale University, New Haven, CT; [3]Vogon Labs, Cochrane, Alberta; [4]Agilent Technologies, Santa Clara, CA*

MOD pm 03:30 **Analysis of yeast lipids exposed to low temperature stress using data-independent acquisition-based lipidomics**; Daiki Hara[1]; Nobuyuki Okahashi[2, 3]; Atsuhiko Toyama[4]; Junko Iida[3, 5]; Fumio Matsuda[2, 3]; *[1]Osaka Univerisity, Suita, Japan; [2]Osaka Univerisity, Suita, Osaka, Japan; [3]Osaka University Shimadzu Omics Innovation Research Laboratories, Suita, Japan; [4]Shimadzu Corporation, Kyoto, Japan; [5]SHIMADZU 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**; Marialuce Maldini[1]; Antonella Chiapparino[2]; Eshani Nandita[3]; *[1]SCIEX, Milano, Italy; [2]SCIEX, Darmstadt, Germany; [3]SCIEX, Redwood City, CA*

MOD pm 04:10 **Plasma Lipidomics using diaPASEF Demonstrates Improved Capabilities of Quantification using MS2 Data**; Premy Shanthamoorthy[1]; Hannes Roest[1]; *[1]University of Toronto, Toronto, ON*

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 Czech[2]; Sven Ehlert[1]; Andreas Walte[1]; Ralf Zimmermann[2, 3]; *[1]Photonion GmbH, Schwerin, Germany; [2]Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; [3]Department for Science and Technology of Life, Light and Matter (LL&M), University of Rostock, Rostock, Germany*

MOE pm 02:50 **Novel mass spectrometry method for the detection and quantification of peanut protein in processed food matrices**; Sara K Schlange[1]; Justin T Marsh[1]; Melanie L Downs[1]; Philip E Johnson[1]; *[1]University 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 Juchelka[3]; Issaku Edward Kohl[3]; Andreas Hilkert[3]; Heiko Hayen[1]; *[1]University of Muenster, Muenster, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo 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 Hu[1]; Miao Yu[2]; Yantao Zhao[1]; Yingdong Zhu[1]; Shengmin Sang[1]; *[1]North Carolina A&T State University, Kannapolis, NC; [2]The 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-Galiano[1]; María José Gómez-Ramos[1]; Icíar Beraza-Gómez[1]; María Murcia-Morales[1]; Amadeo Rodriguez Fernandez-Alba[1]; *[1]University of Almería, Department of Chemistry and Physics, Agrifood Campus of International Excellence (ceiA3), Almeria, 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 Liuu[1]; Kam Eng Trinh[2]; Chenqin Cao[3]; Ekaterina Darii[4]; Annelaure Damont[3]; Jean-Claude Tabet[3, 5]; Yves Gimbert[6]; François Fenaille[3]; Yassine Makni[2]; Chanthadary Inthavong[2]; Gwenaelle LAVISON-BOMPARD[2]; Jacques-Antoine Hennekinne[1]; Olivier Firmesse[1]; *[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]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; [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, Univ Evry, Université Paris-Saclay, Evry, France; [5]Faculté des Sciences et de l'Ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Sorbonne Université, Paris, France; [6]Département de Chimie Moléculaire, UMR CNRS 5250, Université Grenoble Alpes, Grenoble, France*

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 Verzani[1]; Zackery Ely[2]; Karl R Clauser[1]; Susan Klaeger[1]; Zachary Kulstad[2]; Andrew Aguirre[1, 3, 4]; William A Freed-Pastor[2, 4]; Jennifer G Abelin[1]; Tyler Jacks[2]; Steven A Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Massachusetts Institute of Technology, Cambridge, Massachusetts; [3]Harvard Medical School, Boston, MA; [4]Dana-Farber Cancer Institute, Boston, MA*

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 Conrads[3]; 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 Mathiaparanam[1]; Olga Zaslaver[1]; Michelle Kushida[1, 2]; Trevor Pugh[1, 3]; Peter Dirks[1, 2]; J. Rafael Montenegro-Burke[1]; Hannes Röst[1]; *[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 Dehart[1]; Robert A. D'ippolito[1]; Kanika Sharma[1]; Nicole Fer[1]; Brian Smith[1]; Mackenzie Meyer[1]; Scott Eury[1]; Abigail Neish[1]; Katie Powell[1]; Vanessa Wall[1]; William Burgan[1]; Dominic Esposito[1]; Anna E. Maciag[1]; Frank McCormick[1, 2]; Dwight V. Nissley[1]; *[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 Alba[1]; Ielyzaveta Slarve[1]; Brandon Ebright[1]; Whitaker Cohn[2]; Yiren Zhou[1]; Jared Khan[1]; Yunyi Jia[1]; Aditi Datta[1]; Lina He[1]; Taojian Tu[1]; Pranav Pammidimukkala[1]; Phillip Nguyen[1]; Jonathan Katz[1, 3]; Julian Whitelegge[2]; Stan Louie[1]; Bangyan Stiles[1]; *[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 Chaerkady[1]; Li Dai[1]; Kristina Archer[1]; Abby J. Chiang[1]; Lisa H Cazares[1]; Rajat Varma[1]; Mark Cobbold[1]; Sonja Hess[1]; *[1]AstraZeneca R&D, Gaithersburg, Maryland*

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 Eckhoff[1]; Nicholas K. Lubinsky[1]; Luis F. Velasquez-Garcia[1]; *[1]MIT, Cambridge, MA*

MOG pm 02:50 **Real-time Pressure Control Algorithm Enables Vacuum Design for Miniature mass spectrometer**; Ningxi Li[1]; Zhijun Cai[1]; Xiaoyu Zhou[1]; Zheng Ouyang[1]; *[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 Kregel[1]; Blaise J. Thompson[1]; Gilbert M. Nathanson[1]; Timothy H. Bertram[1]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, WI*

MOG pm 03:30 **Mass Spectrometer Observing Lunar Operations (MSolo)**; Roberto Aguilar Ayala[1]; Matthew L. Hancock[1]; Alexander W. Jarnot[1, 2]; Janine E. Captain[1]; Jacqueline W. Quinn[1]; *[1]National Aeronautics and Space Administration, Kennedy Space Center, FL; [2]University of Central Florida, Orlando, FL*

MOG pm 03:50 **Machine learning-derived charge state assignments with better accuracy than human experts**; Heather Desaire[1]; David Hua[1]; Hanna Nguyen[1]; Eden Go[1]; *[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. Miller[1]; Conner C. Harper[1]; Evan R. Williams[1]; *[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**; Weiwen Sun[1]; Yuan Lin[1]; Yue Huang[1]; Josolyn Chan[1]; Sonia Terrillon[1]; Anton I. Rosenbaum[1]; Kevin Contrepois[1]; *[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-Clarke[1]; Tabiwang N. Arrey[2]; Lia Serrano[1]; Noah M Lancaster[1]; Anna Pashkova[2]; Evgenia Shishkova[1]; Michael S. Westphall[1]; Christian Hock[2]; Nicolaie Eugen Damoc[2]; Vlad Zabrouskov[3]; 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 Yu[1]; Ka Yang[1]; Kevin Dong[1]; Martin Zeller[2]; Graeme C McAlister[3]; Joao A Paulo[1]; Hamish Stewart[2]; Christian Hock[2]; Nicolaie Eugen Damoc[2]; Vlad Zabrouskov[3]; Steven P Gygi[1]; *[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 Wen[1]; Kiersten Tovar[1]; Adway O. Zacharias[1]; Chang Liu[2]; Richard Johnstone[1]; Ryan Loy[1]; Lyle Burton[2]; Thomas R. Covey[2]; Markus Koglin[1]; Kevin P. Bateman[3]; Mary Jo Wildey[1]; David G. McLaren[1]; *[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 andComplementaryAnalytical Method for Characterization and Relative Quantitation of Multispecific Antibodies**; Iain D G Campuzano[1]; Fuyi Chen[1]; Dhanashri Bagal[2]; Dwight Winters[1]; Christopher Spahr[1]; Emma Pelegri-O'Day[2]; Nithya Srinivasan[1]; Jennifer L Lippens[1]; Pascal Egea[3]; Aiko Umeda[1]; Jennifer Aral[1]; Tianqi Zhang[4]; Arthur Laganowsky[4]; Marissa Mock[1]; Chawita Netirojjanakul[1]; *[1]Amgen, Thousand Oaks, CA; [2]Amgen, South San Francisco, CA; [3]UCLA, Los Angeles, CA; [4]Texas A&M University, College Station, TX*

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 Kooij[1]; Aleksandra Chojnacka[2]; Garry L. Corthals[2]; Cees Van Rijn[3]; [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 Morgner[1]; Kudratullah Karimi[1]; Jonathan Zöller[2]; Tommy Hofmann[3]; Rene Zangl[1]; Jonathan Schulte[1]; Carla Schmidt[3, 4]; Julian D Langer[2]; [1]*Goethe-University, Insitute 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 Carmany[1]; Paul Demond[2, 3]; Patrick W. Fedick[4]; Elizabeth Dhummakupt[2]; [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 Bautista[1]; Marcos Bouza Areces[2]; Sebastian Brandt[3]; Joachim Franzke[3]; Antonio Molina Díaz[2, 4]; Juan Francisco García Reyes[2, 4]; [1]*Universidad de Jaen, 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 Koss[1]; Matthieu Riva[2]; Felipe Lopez-Hilfiker[2]; [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 Pursell[1]; Liam P. Poole[2]; Kaitlyn J. Apgar[1]; Stephen Valentine[2]; Peng Li[2]; [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 Corveleyn[1]; Lien Provez[2]; Bart Van Puyvelde[1]; Dieter Deforce[1]; Pieter Van Vlierberghe[2]; Maarten Dhaenens[1]; [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. Cunningham[1]; Ellenore P. Craine[1]; Alyssa L. Hansen[1]; Stacy Hall[1]; Dana V. Rizk[1]; Bruce A. Julian[1]; Jan Novak[1]; Matthew B. Renfrow[1]; [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 Tierney[1]; Ting-Wen Cheng[1]; Savon Vigil[1]; Matthew Blatnik[1]; [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 Puyvelde[1]; Christie Hunter[2]; Yang Oliver Wang[3]; Esthelle Hoedt[3]; Maxim Zhgamadze[3]; Koen Raedschelders[3]; Qin Fu[3]; Dieter Deforce[1]; Maarten Dhaenens[1]; Jennifer Van Eyk[3]; [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 Chen[1]; Cindy J. Lee[1]; Stanislav S. Rubakhin[1]; Jonathan V. Sweedler[1]; [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 Fahrmann[1]; Ehsan Irajizad[1]; Jody Vykoukal[1]; Angelica Gutierrez Barrera[1]; Jennifer B Dennison[1]; Ranran Wu[1]; Banu Arun[1]; Abenaa Brewster[1]; Samir Hanash[1]; [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 Zhao[1]; Carter Lantz[1]; Benqian Wei[1]; Rachel R. Ogorzalek Loo[1]; Joseph A. Loo[1]; [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 Wang[3]; [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-Nissan[1]; David Morgenstern[1]; Yegor Leushkin[1]; Michal Sharon[1]; [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 Yin[1]; Janet C Saunders[2]; Paul WA Devine[2]; Nicholas J Bond[2]; Albert J.R. Heck[1]; [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 Marie[1]; Somak Ray[1]; Alexander R. Ivanov[1]; [1]*Barnett Institute of Chemical and Biological Analysis, Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA*

TOC am 10:10 **In-Line Soft Landing for Cryo-EM and Mass Spectrometry Characterization of Hydrated Native Complexes and Glycoproteins**; Elizabeth Duselis[1]; Henry Benner[2]; Ben Aguilar[2]; Ananya Dubey Kelsoe[2]; Matthew Johnson[1]; Wayne Fairbrother[1]; Alexis Rohou[1]; Elizabeth Hecht[1]; *[1]Genentech, South San Francisco, CA; [2]IonDX 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 Shannon[1]; Damien B Wilburn[1]; *[1]The Ohio State University, Columbus, OH; [2]Proteome Software, Portland, OR*

TOD am 08:50 **A systematic characterization of LC-MS features sheds light on the full potential of DIA identification**; Grzegorz Skoraczyński[1]; Tejas Gandhi[1]; Oliver M Bernhardt[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

TOD am 09:10 **Library-free analysis of DIA experiments using a feature-centric approach**; J. Sebastian Paez[1]; Carolyn Allen[1]; Lindsay K Pino[1]; Daniele Canzani[1]; William E Fondrie[1]; *[1]Talus Bioscience, Seattle, WA*

TOD am 09:30 **Fragment ion intensity prediction improves the identification rate of non-tryptic peptides in TimsTOF**; Charlotte Adams[1]; Wassim Gabriel[2]; Kris Laukens[1]; Wout Bittremieux[1]; Mathias Wilhelm[2]; Kurt Boonen[1]; *[1]University of Antwerp, Antwerpen, Belgium; [2]Technical University of Munich, Munich, Germany*

TOD am 09:50 **A modular and open workflow for the extraction and quantificationof peptides in synchro-PASEF experiments**; Georg Wallmann[1]; Patricia Skowronek[2]; Marvin Thielert[2]; Corazon Ericka Mae Itang[1]; Sander Willems[3, 4]; Wen-Feng Zeng[1]; Matthias Mann[1, 5]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Max Planck Institute of Biochemistry, Martinsried, Germany; [3]Max Planck Institute of Biochemistry, Planegg, Germany; [4]Bruker Daltonics, Bremen, Germany; [5]NNF Center for Protein Research, University of Copenhagen, Copenhagen, Denmark*

TOD am 10:10 **SEPepQuant 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]; *[1]Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; [2]Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, 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 Zhao[1]; Wout Bittremieux[1, 2]; Corinna Brungs[3]; Robin Schmid[1, 3]; Simone Zuffa[1]; Pieter C Dorrestein[1]; *[1]University of California San Diego, San Diego, CA; [2]University of Antwerp, Antwerpen, Belgium; [3]Institute 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 McKeon[1]; Chiara Lecchi[1]; Peter W. Villalta[1]; Silvia Balbo[1]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, MN; [2]Center 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 Smith[1]; Robert N O'Meally[2]; Sean M Burke[1]; Robert H Brown[1, 3]; John D Groopman[1]; Robert N Cole[2]; *[1]Department of Environmental Health and Engineering, Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD; [2]Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD; [3]Department of Anesthesiology, School of Medicine, Johns Hopkins University, Baltimore, MD*

TOE am 09:50 **Chemical exposome in brain cancer: An exploratory study**; Ruben Gil-Solsona[1]; Albert Pons-Escoda[2]; Daniel Gutierrez-Martin[1]; Jordi Bruna[3, 3]; Noemi Vidal-Sarro[4]; Carles Majos[2]; Pablo Gago Ferrero[1]; *[1]Institute of Environmental Assessment and Water Research - Spanish Council for Scientific Research (IDAEA-CSIC), Barcelona, Spain; [2]Department of Neuroradiology, Hospital Universitari de Bellvitge, C. Feixa Llarga SN, 08907 L'Hospitalet de Llobregat, Spain, Hospitalet de Llobregat, Spain; [3]Unit of Neuro-Oncology. Hospital Universitari de Bellvitge-ICO, Barcelona, Spain; [4]; Neuropathology 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 Beres[1]; Sarah Doydora[2]; Kaylie I Kirkwood[3]; Allen Li[4]; Owen Duckworth[2]; Erin S Baker[1]; *[1]Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Department of Crop and Soil Sciences, North Carolina State University, Raleigh, NC; [3]Department of Chemistry, North Carolina State University, Raleigh, NC; [4]Institute 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 Wang[1]; Ping-Chung Chen[1]; Junmin Peng[1]; *[1]St. 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 Pathmasiri[1]; Stephanie M Cologna[1]; *[1]University 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 Leontyev[1]; Alexis N Pulliam[2]; David A Gaul[1]; Michelle C Laplaca[2]; Facundo M Fernandez[1]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; [2]Coulter 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**

Disease; Yun Tang[1]; Hyejin Park[1]; Michael C. Fitzgerald[1]; *[1]Duke University, Durham, NC*

TOF am 09:50 **BrainProt: An Omics based knowledgebase towards the understanding of Human Brain and diseases**; Deeptarup Biswas[1]; Sanjyot Vinayak Shenoy[1]; Aparna Chauhan[1]; Advait Padhye[1]; Sanjeeva Srivastava[1]; *[1]IIT 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. Alvarez[2]; Ryan Lee Schindler[2]; Armin Oloumi[2]; Tristan Alexander Seales[2]; Siyu Chen[2]; Nikita P. Bacalzo, Jr. [2]; Jorge Gil C. Angeles[1]; Francisco M. Heralde III[3]; Jomar F. Rabajante[1]; Ruel C. Nacario[1]; Gladys C. Completo[1]; Carlito B. Lebrilla[2]; *[1]University of the Philippines Los Banos, Los Banos, Laguna, Philippines; [2]University of California, Davis, Davis, CA; [3]University 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 Bateman[1]; Fabien Fontaine[2]; Bernard Choi[1]; Luca Morettoni[3]; Ismael Zamora[2]; *[1]Preclinical Development, Merck Research Lab. Merck & Co., Inc, West Point, PA; [2]Lead Molecular Design, S.L., Sant Cugat del Valles, Spain; [3]Molecular 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 Baghla[1]; Eshani Nandita[1]; *[1]SCIEX, 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 Dong[1]; Julie Lade[1]; Fang Xie[1]; Zhe Wang[1]; Xiaomeng Shen[1]; *[1]Amgen, 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 Laux[1]; Stefan Blech[2]; *[1]Boehringer Ingelheim Pharma, Biberach, Germany; [2]Boehringer 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 Hossain[1]; Rutali R. Brahme[1]; Brandon C. Miller[1]; Jakal Amin[1]; Jared R. Auclair[1]; Qingping Wang[2]; David J. Greenblatt[3]; Roman Manetsch[1]; Jeffrey N. Agar[1]; *[1]Northeastern University, Boston, MA; [2]Sanofi, Cambridge, MA; [3]School of Medicine, Tufts University, Boston, MA*

TOG am 10:10 **Quantitative Proteomics supports characterization of complex translational in vitro models for oral prodrugs**; Xue Wang[1]; Liang Jin[1]; Abhinav Sharma[2]; David Stresser[2]; Yu Tian[1]; *[1]AbbVie Bioresearch Center, Worcester, MA; [2]AbbVie 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 Zemaitis[1]; Dušan Veličković[1]; David J Degnan[1]; James M Fulcher[1]; Lye Meng Markille[1]; Yu Mi Kwon[1]; Dehong Hu[1]; Yen-Chen Liao[1]; Sarah M Williams[1]; Lisa M Bramer[1]; Ying Zhu[1]; William Kew[1]; Wei-Jun Qian[1]; Mowei Zhou[1]; Ljiljana Paša-Tolić[1]; *[1]Pacific 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. Schurman[1]; Nannan Tao[2]; Jonathon J. Woo[3]; Tamara Alliston[3]; Peggi M. Angel[4]; Birgit Schilling[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]Bruker Daltonics, San Jose, CA; [3]University of California San Francisco, Department of Orthopaedic Surgery, San Francisco, CA; [4]Medical 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 Schweizer[1]; Rahul Krishnan[2]; Aasa Shimizu[2]; Andreas Metousis[1]; Hilary Kenny[2]; Lisha Zhu[3]; Thierry Nordmann[1]; Florian Rosenberger[1]; Agnes Julia Bilecz[4]; Rachelle Mendoza[4]; Sanaa Nakad Borrego[2]; Marvin Thielert[1]; Sophia Mädler[1]; Andreas Mund[5]; Mengjie Chen[3]; Ricardo Lastra[4]; Matthias Mann[1, 5]; Ernst Lengyel[2]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Department of Obstetrics and Gynecology/Section of Gynecologic Oncology, University of Chicago, Chicago, Illinois; [3]Medicine/Section of Genetic Medicine, The University of Chicago, Chicago, Illinois; [4]Department of Pathology, The University of Chicago, Chicago, Illinois; [5]Proteomics 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-Deschmann[1]; Martin Handelshauser[1]; Aleksandra Lebedeva[1]; Orestis Andriotis[1]; Philipp Thurner[1]; *[1]TU Wien, Vienna, Austria*

TOH am 09:50 **MALDI Imaging of Post-Mortem COVID-19 Lungs**; Caitlin Tressler[1]; Gargey B. Yagnik[2]; Karl Smith[3, 4]; Nicole M. Jenkinson[1]; Chad Weisbord[4]; Kenneth J. Rothschild[2]; Mark J. Lim[2]; David Nauen[1]; Kristine Glunde[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD; [2]AmberGen, Inc., Billerica, MA; [3]Leibniz-Institut für Analytische Wissenschaften—ISAS—e.V., Dortmund, Germany; [4]National High Magnetic Field Laboratory, Tallahassee, FL*

TOH am 10:10 **Software workflow and statistical analysis tools for evaluating multiomics MALDI MSI studies**; Tobias Boskamp[1]; Sören-Oliver Deininger[1]; Mark Lim[2]; Gargey Yagnik[2]; Nathalie Agar[3]; Sylwia Stopka[3]; Richard R. Drake[4]; Stacy A. Malaker[5]; Rachel Stubler[4]; Kenneth J. Rothschild[2, 6]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]AmberGen, Inc., Billerica, MA; [3]Harvard Medical School, Boston, MA; [4]Medical University of South Carolina, Charleston, SC; [5]Yale University, New Haven, CT; [6]Boston 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 Johnson[1]; Martin E. Palmer[1]; Peter Nixon[1]; Jason Wildgoose[1]; *[1]Waters 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. Heil[1]; Nicolaie Eugen Damoc[2]; Tabiwang N. Arrey[2]; Anna Pashkova[2]; Chris Hsu[1]; Christine C. Wu[1]; Philip M Remes[3]; Hamish Stewart[2]; Christian Hock[2]; Michael Senko[3]; Vlad Zabrouskov[3]; Michael J. MacCoss[1]; *[1]University of Washington, Seattle, WA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo 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 Wootton[1]; Alina Theisen[1]; Gregory Brabeck[1]; Carlos Schat[1]; Claudia Kriete[1]; Roland Jertz[1]; *[1]Bruker Daltonics, Bremen, Germany*

TOA pm 03:30 **High Resolution Analysis of Megadalton Sized DNA using Charge Detection Mass Spectrometry**; Lohra Miller[1]; Polycarp Ooegbu[1]; Benjamin Draper[1]; Martin F. Jarrold[1]; *[1]Indiana University Bloomington, Bloomington, IN*

TOA pm 03:50 **A novel quaternary hybrid Q-Orbitrap-IT-FT-ICR mass spectrometry platform**; Chad R. Weisbrod[1]; Jesse D. Canterbury[2]; John P Quinn[1]; Lissa C Anderson[1]; Amy M McKenna[1]; Greg T Blakney[1]; Michael W. Senko[2]; Christopher L. Hendrickson[1]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Thermo 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 Ray[1]; Ricardo Arevalo, Jr. [3]; Ryan M. Danell[2, 4]; Jacob D Graham[2]; Andrej Grubisic[2]; Cynthia L Gundersen[5]; Niko A Minasola[5]; Anthony W Yu[2]; Molly E Fahey[2]; Christelle Briois[6]; Laurent Thirkell[6]; Fabrice Colin[6]; *[1]University of Maryland College Park, College Park, MD; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]University of Maryland, College Park, College Park, MD; [4]Danell Consulting, Winterville, NC; [5]AMU Engineering, Miami, FL; [6]LPC2E, 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. Arrey[3]; Anna Pashkova[3]; Nicholas Arp[4, 5]; Jing Fan[4, 5, 6]; Evgenia Shishkova[2, 7]; Michael S. Westphall[2, 7]; Hamish Stewart[3]; Eugen Damoc[3]; Vlad Zabrouskov[8]; Joshua J. Coon[1, 2, 4, 7]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Morgridge Institute for Research, Madison, WI; [5]Cellular and Molecular Biology Graduate Program, University of Wisconsin-Madison, Madison, WI; [6]Department of Nutritional Sciences, University of Wisconsin-Madison, Madison, WI; [7]National Center for Quantitative Biology of Complex Systems, Madison, WI; [8]Thermo 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 Caefer[1]; Jeremy Balsbaugh[1]; Jennifer Liddle[1]; Anastasios Tzingounis[1]; Daniel Schwartz[1]; *[1]University of Connecticut, Storrs, CT*

TOB pm 03:10 **Investigating T-cell Activation Using the Phosphorylation Integrated Thermal Shift Assay**; Brandon M Gassaway[1]; Alison E. Ringel[2]; Emily M. Huntsman[3]; Jared L. Johnson[3]; Lewis C. Cantley[3]; Edward L Huttlin[1]; Steven P Gygi[1]; Marcia C. Haigis[1]; *[1]Harvard Medical School, Boston, MA; [2]MIT, Cambridge, MA; [3]Weill Cornell Medicine, New York, NY*

TOB pm 03:30 **Time-resolved deep ubiquitinome profiling for protein degraders**; Ishwar Kohale[1]; Aman Makaju[2]; Han-Yin Yang[1]; Bradford Gibson[1]; Daryl N Bulloch[1]; *[1]Amgen, South San Francisco, CA; [2]Amgen, Thousand Oaks, CA*

TOB pm 03:50 **A quantitative and site-specific atlas of the in vivo citrullinome reveals widespread existence of citrullination**; Alexandra Stripp[1]; Ivo A Hendriks[1]; Sara C Buch-Larsen[1]; Jonas D Elsborg[1]; Rebecca Kirsch[1]; Nadezhda T Doncheva[1]; Lars J Jensen[1]; Maria Christophorou[2]; Michael L Nielsen[1]; *[1]NNF Center for Protein Research, Univ of Copenhagen, Copenhagen N, Denmark; [2]Babraham Institute, Cambridge, United Kingdom*

TOB pm 04:10 **PTMeXchange : Globally harmonized re-analysis and sharing of data on post-translational modifications**; Kerry A Ramsbottom[1]; Oscar M Camacho[1]; Zhi Sun[2]; Emily Bowler-Barnett[3]; Jun Fan[3]; Ananth Surappa-Narayanappa[3]; Deepti Kundu[3]; Yasset Perez-Riverol[3]; Maria-Jesus Martin[3]; Juan Antonio Vizcaino[3]; Eric W. Deutsch[2]; Andrew R Jones[1]; *[1]University of Liverpool, Liverpool, United Kingdom; [2]Institute for Systems Biology, Seattle, WA; [3]EMBL'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 Hanozin[1]; Conner C Harper[1]; Matthew S. McPartlan[1]; Evan R. Williams[1]; *[1]University 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 Cordes[1]; Elyssia S. Gallagher[1]; *[1]Baylor University, Waco, TX*

TOC pm 03:10 **Transition metal identification and speciation by MALDI FT-ICR MS as salen complexes**; Elena Giaretta[1]; Farah Salma[1, 2]; Davide Corinti[3]; Caterina Bordin[1]; Manal Ridany[1]; Mariaelisa Crestoni[3]; Christian Rolando[1, 4]; *[1]Faculty of Sciences & Technologies, University of Lille, Villeneuve d'Ascq, France; [2]Faculty of Science III, Lebanese University, Tripoli, Lebanon; [3]Dipartimento di Chimica e Tecnologie del Farmaco, Sapienza - Università di Roma, Roma, Italy; [4]Shrieking Sixties - 1-3 Allée Lavoisier, Villenueve d'Ascq, France*

TOC pm 03:30 **Effect of gas-phase on reactant ions, ionization and fragmentation in dielectric barrier discharge**

ionization; Markus Weber[1, 2]; Christoph Haisch[2]; Jan-Christoph Wolf[1]; [1]*Plasmion GmbH, Augsburg, Germany;* [2]*Technical University of Munich, Munich, Germany*

TOC pm 03:50 **Unravelling the Mechanisms of Magic Number Custer Formation During Electrospray Ionization**; Lars Konermann[1]; Yousef Haidar[1]; Vida Alinezhad[1]; Elnaz Aliyari[1]; [1]*Univ. of Western Ontario, London, ON*

TOC pm 04:10 **Use of Acoustic Energy to Disrupt Exosomes for Direct Compositional Analysis by MS**; Ashton N Taylor[1]; Cheyenne Sircher[1]; Yuqi Huang[1]; Venkat Bhethanabotla[1]; Theresa Evans-Nguyen[1]; [1]*University of South Florida, Tampa, FL*

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 Shen[1]; Ryan Kellogg[1]; Daniel Panyard[1]; Nasim Bararpour[1]; Kevin Castillo[1]; Brittany Lee-McMullen[1]; Alireza Delfarah[1]; Jessalyn Ubellecker[1]; Sara Ahadi[1]; Yael Rosenberg-Hasson[1]; Ariel Ganz[1]; Kevin Contrepois[1]; Basil Michael[1]; Ian Simms[1]; Chuchu Wang[1]; Daniel Hornburg[1]; Michael Snyder[1]; [1]*Stanford 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]; [1]*VIB-UGent Center for Medical Biotechnology, Ghent, Belgium;* [2]*Department of Biomolecular Medicine, Faculty of Health Sciences and Medicine, Ghent, Belgium;* [3]*Interuniversity Institute of Bioinformatics in Brussels, ULB-VUB, Brussels, Belgium;* [4]*Structural 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 Hao[1]; Jessica Roberts[1]; Rahel Bezabih[1]; Mark R. Cookson[3]; Michael E. Ward[4]; Andrew B. Singleton[1]; Mike A. Nalls[1, 2]; Yue A. Qi[1]; [1]*Center for Alzheimer's and Related Dementias, National Institutes of Health, Bethesda, MD;* [2]*Data Tecnica International, Washington, DC;* [3]*Laboratory of Neurogenetics, National Institute on Aging, National Institutes of Health, Bethesda, MD;* [4]*National 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 Pergande[1]; Yutong Jin[1]; Kalina J Rossler[1]; Gary M Diffee[1]; Rozalyn M Anderson[1]; Ricki J Colman[1]; Ying Ge[1]; [1]*University of Wisconsin-Madison, Madison, WI*

TOD pm 03:50 **Development of a Tumor Immunopeptidome database for T cell-based therapies**; Yulun Chiu[1]; Ke Pan[1]; Cassian Yee[1]; [1]*The 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 Cox[1]; Joshua J. Coon[2, 3, 4, 7]; [1]*Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Martinsried, Germany;* [2]*Morgridge Institute for Research, Madison, WI;* [3]*National Center for Quantitative Biology of Complex Systems, Madison, WI;* [4]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [5]*EMBL Australia and Garvan Institute of Medical Research, Darlinghurst, Australia;* [6]*School of Biotechnology and Biomolecular Sciences, University of New South Wales, Sydney, Australia;* [7]*Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI;* [8]*Department of Microbiology and Ecosystem Science, University of Vienna, Vienna, Austria;* [9]*Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON;* [10]*Department of Molecular Genetics, University of Toronto, Toronto, ON*

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 Santos[1]; Nerilson M Lima[1]; Gesiane S Lima[1]; Jussara V Roque[1]; Gagan Preet[2]; Teresinha De Jesus A. S. Andrade[3]; Marcel Jaspars[4]; Boniek Gontijo[1]; [1]*Federal University of Goiás - UFG, Goiânia, Brazil;* [2]*University of Aberdeen, Aberdeen Proving Ground, United Kingdom;* [3]*GEOMAR Helmholtz Centre for Ocean Research Kiel, Kiel, Germany;* [4]*federal 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 Popowich[1]; Jose Luis Lazarte Luna[1]; Catherine Gilbert[2]; Monica Katz[3]; Ronda Kasl[1]; Christopher Mason[4]; Caroline Tokarski[2]; Julie Arslanoglu[1]; [1]*Metropolitan Museum of Art, New York, NY;* [2]*Institute of Chemistry and Biology of Membrane and NanoObjects (CBMN), CNRS UMR 5248 University of Bordeaux, Bordeaux, France;* [3]*The Hispanic Society of America, New York, NY;* [4]*Weill 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 Behsaz[1]; Andrés Mauricio Caraballo-Rodríguez[2]; Pieter C Dorrestein[2]; Hosein Mohimani[1]; [1]*Carnegie Mellon University, Pittsburgh, PA;* [2]*University 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 Nyarko[1]; Kaitlyn Boozer[1]; Michael Greenlief[1]; [1]*University 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 Williams[1]; James M Fulcher[1]; William Chrisler[1]; Liyu Andrey[1]; Lye Meng Markille[1]; Vimal Kumar Balasubramanian[1]; Mowei Zhou[1]; Jaeho Song[2]; Gary Stacey[2]; Amy Marshall-Colon[3]; John Mullet[4]; Amirhossein H. Ahkami[1]; Ljiljana Pasa-Tolic[1]; Ying Zhu[5]; [1]*Pacific Northwest National Laboratory, Richland, WA;* [2]*University of Missouri, Columbia, MO;* [3]*University of Illinois at Urbana-Champaign, Urbana, IL;* [4]*Texas A&M University, College Station, TX;* [5]*Genentech 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 Bartels[1]; Erbil Güngör[2]; Sara Tortorella[3]; Ismael Zamora[4]; Henriette Schluepmann[2]; Ron M.a.

Heeren[1]; 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 Kit[1]; Tyler C Cropley[2]; Frank Sobott[3]; Christian Bleiholder[2]; Ian K. Webb[1]; *[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-Younis[1]; Alexander Zhyvoloup[1]; Hannah Britt[1]; Daniel Raleigh[1, 2]; Konstantinos Thalassinos[1]; *[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 Henderson[1]; Edie M. Sharon[1]; Adam J Anthony[1]; Sarah M. O'keefe[1]; David E. Clemmer[1]; *[1]Indiana University Bloomington, Bloomington, IN*

TOF pm 03:30 **Ion Mobility – Mass SpectrometryEvaluates the Effects of Lipid Bilayers On Membrane Protein Structure and Stability**; Iliana Levesque[1]; Aniruddha Panda[2]; Kallol Gupta[2]; Brandon T Ruotolo[1]; *[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 Blanksby[1]; Berwyck Poad[1]; Reuben S. E. Young[1, 2]; Lachlan Jekimovs[1]; Felicia Hansen[1]; Thi Phuong Do[1]; Hendrik Frisch[1]; Michael Pfrunder[1]; David L Marshall[1]; Kathleen Mullen[1]; *[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 Dieke[1]; Joshua Shipman[1]; Cynthia Sommers[1]; Jason Rodriguez[1]; Deyi Zhang[2]; Darby Kozak[2]; Kui Yang[1]; *[1]U.S. Food and Drug Administration, Saint Louis, MO; [2]U.S. Food and Drug Administration, Silver Spring, MD*

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 Lin[1]; Patrick Haller[1, 2]; Navid Bavi[1, 2]; Nabil Faruk[1]; 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**; Yuqi Shi[1]; Hariharan Parameswaran[2]; Lan Guan[2]; Rosa Viner[1]; *[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. Quintero[1]; O. Tara Liyanage[1]; Elyssia S. Gallagher[1]; *[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 Kish[1]; Dylan P Ivory[1]; Jonathan J Phillips[1]; *[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 Wu[1]; Mulin Fang[1]; Kellye A. Cupp-Sutton[1]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK*

TOG pm 04:10 **Selective protein capture under HDX-MS quench conditions for probing complex biological systems**; Dietmar Hammerschmid[1]; Anthony Keeble[2]; Polina Heatley[1]; Mark Howarth[2]; Eamonn Reading[1]; *[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-Tawiah[1]; Ayesha Seth[2]; Muralikrishnan Girish[2]; Kingsley Badu[3]; *[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. Chace[1]; Daniel Magiera[2]; Nesta Bortey-Sam[3]; Jerry Vockley[4]; *[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 Zecha[1]; Junmin Wang[2]; Stefani N. Thomas[3]; Ventzislava A. Hristova[1]; Sonja Hess[1]; *[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 Whiteaker[1]; Lei Zhao[1]; Uliana Voytovich[1]; Jacob J. Kennedy[1]; George Miles[2]; Galen Hostetter[3]; Chelsea Newton[3]; Scott Jewell[3]; Yongchao Dou[2]; Yuxing Liao[2]; Bing Zhang[2]; Andy

Hoofnagle[4]; Shrabanti Chowdhury[5]; Pei Wang[5]; Amanda G. Paulovich[1]; *[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 Merrigan[1]; Preejith P. Vachali[1]; Elizabeth L. Frank[2]; *[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 Liscio[3]; Steven Corless[1]; Patrick Sears[2]; Chris Hopley[1]; *[1]LGC, Teddington, United Kingdom; [2]University of Surrey, Guildford, United Kingdom; [3]Element Materials Technology, Cambridge, United Kingdom*

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. Kozhinov[1]; Konstantin O. Nagornov[1]; Camille Garcia[2]; Tingting Fu[2]; Julia Chamot-Rooke[2]; Yury O. Tsybin[1]; *[1]Spectroswiss, Lausanne, Switzerland; [2]Mass 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 Butalewicz[1]; Edwin Escobar[1]; Christopher A. Wootton[2]; Melvin A Park[3]; Erin H. Seeley[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bruker Daltonics, Billerica, MA*

WOA am 09:10 **Adding a cryogenic IR spectroscopic dimension to LC-MS**; Ali H. Abikhodr[1]; Stephan Warnke[1]; Ahmed Ben Faleh[1]; Thomas Rizzo[1]; *[1]Ecole 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 Makarov[1]; Christian Hock[1]; Hamish Stewart[1]; Dmitry Grinfeld[1]; Anastassios Giannakopulos[1]; Johannes Petzoldt[1]; Toby Shanley[1]; Eduard Denisov[1]; Amelia Peterson[1]; Matthew Garland[1]; Nicolaie Eugen Damoc[1]; Martin Zeller[1]; Tabiwang N. Arrey[1]; Anna Pashkova[1]; Andreas Kuehn[1]; Matthias Biel[1]; Arne Kreutzmann[1]; Bernd Hagedorn[1]; Immo Colonius[1]; Adrian Schuetz[1]; Arne Stefes[1]; Ankit Dwivedi[1]; Daniel Mourad[1]; Max Hoek[1]; Philipp Cochems[1]; Alexander Kholomeev[1]; Robert Ostermann[1]; Gregor Quiring[1]; Maximilian Ochmann[1]; Sascha Moehring[1]; Alexander Wagner[1]; Andre Petker[1]; Sebastian Kanngiesser[1]; Michael Wiedemeyer[1]; Wilko Balschun[1]; Frank Czemper[1]; Vlad Zabrouskov[2]; Daniel Hermanson[2]; Andreas Wieghaus[1]; Jean-Jacques Dunyach[2]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo 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. Cabrera[1]; Brian H. Clowers[1]; *[1]Washington 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 Fan[1]; Zi Yang[2, 3]; Xiao Fan[2, 3]; Hongwei Wang[2, 3]; Xiaoyu Zhou[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Department of Precision Instrument, Beijing, China; [2]Tsinghua University, Beijing, China; [3]Tsinghua-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 Liuqing Shi[1]; Michael A. Dillon[1]; Philip D. Compton[2]; Christoph Spiess[1]; Jonathan L. Josephs[1]; John C. Tran[1]; *[1]Genentech Inc, South San Francisco, CA; [2]Integrated 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 Chen[1]; Harsha P. Gunawardena[2]; Yongling Ai[1]; Jinshan Gao[3]; Richard N Zare[4]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]Janssen Research & Development, Spring House, PA; [3]Montclair State University, Montclair, NJ; [4]Stanford University, Stanford, CA*

WOB am 09:10 **The Use of Mass Spectrometry in Therapeutic Protein Biologics License Applications: A Retrospective Review Revisited**; Jamie Mans[1]; Mercy Oyugi[2]; Bethel Asmelash[1]; Cynthia Sommers[1]; Sarah Rogstad[2]; *[1]US Food and Drug Administration, Saint Louis, MO; [2]US 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 Smith[1]; Sara Carillo[1]; Kristina Srzentić[2]; Tabiwang N. Arrey[2]; Anna Pashkova[3]; Kai Scheffler[3]; Kelly Broster[4]; Nicolaie Eugen Damoc[2]; Jonathan Bones[1, 5]; *[1]The National Institute for Bioprocessing Research & Training, Mount Merrion, Ireland; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, Reinach, Switzerland; [4]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [5]University 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. Botamanenko[1]; Benjamin E. Draper[1]; Martin F. Jarrold[2]; *[1]Megadalton Solutions, Bloomington, IN; [2]Indiana 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 Dawdy[1]; Brian C Gau[1]; Leah Hanliu Wang[1]; Carlos H Castaneda[1]; Olga V Friese[1]; Matthew S Thompson[2]; Thomas F Lerch[1]; David J Cirelli[2]; Jason C Rouse[2]; *[1]Pfizer, Chesterfield, MO; [2]Pfizer, 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 celluar pathways following MARC1 knockdown in mouse models of NASH**; David Chow[1]; Yuanjun Guo[1]; Edward Lagory[1]; Han-Yin Yang[1]; Bradford Gibson[1]; Matthew Rardin[1]; *[1]Amgen, Inc., South San Francisco, CA*

WOC am 08:50 **Deciphering Deubiquitinase Ubiquitin Signaling and Substrate Degradation by DIA-PASEF**; He Zhu[1]; Guillaume Adelmant[2]; Indrajit Sahu[2]; Nouf Alharbi[2]; Ujwal Punyamurtula[2]; Scott B. Ficarro[2]; Sara J. Buhrlage[3]; Jarrod A. Marto[2]; *[1]Dana-Farber Cancer Institute, Boston, MA; [2]Department of Cancer Biology, Department of Oncologic Pathology, Blais Proteomics Center, Dana-Farber Cancer Institute, Boston, MA; [3]Department 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 Walker[1]; José Luis Marín-Rubio[1]; Frank H. Büttner[2]; Matthias Trost[1]; Maria Emilia Dueñas[1]; *[1]Biosciences Institute Faculty of Medical Sciences, Newcastle University, NE2 4HH, Newcastle Upon Tyne, United Kingdom;*

[2]*Drug Discovery Sciences, Boehringer Ingelheim Pharma GmbH & Co. KG, Birkendorfer Str. 65, Biberach an der Riß, Germany*

WOC am 09:30 **Simultaneous In situ Pharmacological Profiling of Transcription Factors for Cancer Therapy**; Lindsay K Pino[1]; Andrea Gutierrez[1]; Julia E Robbins[1]; Carolyn Allen[1]; Erin Broderick[1]; Tonibelle Gatbonton-Schwager[1]; Brian McEllin[1]; Sebastian Paez[1]; Yang Gao[1]; William E Fondrie[1]; Daniele Canzani[1]; Alexander Federation[1]; [1]*Talus Bioscience, Seattle, WA*

WOC am 09:50 **Employing mass spectrometry and positional peptide patterns to probe for bioactive peptides**; Christian T Madsen[1]; Jan C. Refsgaard[1]; Felix G. Teufel[1]; Sonny K. Kjærulff[1]; Zhe Wang[2]; Guangjun Meng[2]; Carsten Jessen[1]; Petteri Heljo[1]; Qunfeng Jiang[2]; Xin Zhao[2]; Bo Wu[2]; Xueping Zhou[2]; Yang Tang[2]; Jacob F. Jeppesen[1]; Christian D. Kelstrup[1]; Stephen T. Buckley[1]; Søren Tullin[1]; Jan Nygaard-Jensen[1]; Xiaoli Chen[2]; Fang Zhang[2]; Jesper V. Olsen[3]; Dan Han[2]; Mads Grønborg[1]; Ulrik De Lichtenberg[4]; [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 Fontaine[1]; Tatiana Radckenko[1]; Paula Cifuentes[1]; Albert Garriga[1]; Xavier Pascual[1]; Luca Morettoni[2]; Nadia Zara[2]; Ismael Zamora[1]; [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 Patel[1]; Ramon Adalia[2]; Anthony Paiva[1]; Ismael Zamora Rico[2]; Wilson Shou[1]; Xianmei Cai[1]; Tierni Kaufman[3]; [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 Remes[1]; Jesse Canterbury[1]; William Barshop[1]; Lilian Heil[2]; Cristina Jacob[1]; Michael J. MacCoss[2]; [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 Yilmaz[1]; William E Fondrie[2]; Wout Bittremieux[3]; Rowan Nelson[1]; Varun Ananth[1]; Sewoong Oh[1]; William S Noble[1]; [1]*University of Washington, Seattle, WA;* [2]*Talus Bioscience, Seattle, WA;* [3]*University of Antwerp, Antwerpen, Belgium*

WOD am 09:30 **Improving Peptide Identification Rate by Machine Learning with Second-Ranked Peptide Spectrum Matches**; Johra Muhammad Moosa[1]; 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 Wilburn[1]; Brian C. Searle[2]; [1]*Ohio State University, Columbus, OH;* [2]*The Ohio State University-Comprehensive Cancer Center, Colombus, OH*

WOD am 10:10 **Real-time Analysis and Classification of Aerosol Particles using Single-Particle Mass Spectrometry and Machine Learning**; Heinrich Ruser[1]; Guanzhong Wang[1]; Julian Schade[2, 3]; Johannes Passig[3]; 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-Gonzalez[1]; Dujuan Lu[1]; Chongming Liu[1]; Danny Hower[1]; Aaron Lamb[2]; Jon Bardsley[2]; Min Du[3]; Sven Hackbusch[4]; [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 Yoo[1]; Hugh E. Jones[1]; Mark P. Barrow[1]; Diana Catalina Palacio Lozano[1]; [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 Heimbach[1]; David Light[1]; Kaury Kucera[1]; Mara Dubnicka[1]; Leslie Silva[2]; [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 Lam[1]; Mohamed Hemida[1]; Navneet Singh[2]; Matthew Askeland[2]; Pawel Kidon[2]; Fraser Smith[1]; Andrew Gooley[1]; [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 Räss[1]; Sandra Schaer[1]; Marco Tognetti[1]; Roland Bruderer[1]; Lukas Reiter[1]; [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. Muehlbauer[1]; Mark A. Strege[1]; Trent J. Oman[1]; Donald S. Risley[1]; Ankur Jalan[1]; Zhirui Lian[1]; [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**

Mobility; Komal Kedia[1]; Rachel Harris[2]; Kim Ekroos[3]; Kevin P. Bateman[4]; *[1]Merck, west point, PA; [2]MOBILion Systems, Chadds Ford, PA; [3]Lipidomics Consulting Ltd., Irisviksvägen 31D 02230, Finland; [4]Merck, West Point, PA*

WOF am 08:50 **Spatially and temporally probing distinctive phospholipid alteration in Alzheimer's disease mouse brain via high-resolution ion mobility-enabled sn-position resolved lipidomics**; Shuling Xu[1]; Zhijun Zhu[1]; Daniel G. Delafield[1]; Michael J. Rigby[1]; Luigi Puglielli[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WOF am 09:10 **In-Situ Droplet-Based Tissue Derivatization for Lipid Isomer Characterization Using LESA**; Dallas P. Freitas[1]; Xi Chen[1]; Erin A. Hirtzel[1]; Madison E. Edwards[1]; Joohan Kim[1]; Hongying Wang[1]; Yuxiang Sun[1]; Klaudia I. Kocurek[1]; David Russell[1]; Xin Yan[1]; *[1]Texas A&M, College Station, TX*

WOF am 09:30 **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 Caestecker[6]; 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; [6]Division 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 Ledoux[1]; Yanis Zirem[2]; Florence Renaud[3]; Michel Salzet[2]; Isabelle Fournier[2]; *[1]Laboratoire PRISM - Université de Lille, Villeneuve d'ascq, France; [2]PRISM Inserm U1192 - University of Lille, Villeneuve D'ascq Cedex, France; [3]UMR-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 Fiorante[1]; Michael Woolman[1]; David Munoz[1]; Gelareh Zadeh[1]; Sunit Das[1]; Howard Ginsberg[1]; Arash Zarrine-Afsar[1]; *[1]University of Toronto, Toronto, ON*

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 Jochem[1]; Anna Schrempf[2]; Lina-Marie Wagner[1]; Georg Winter[2]; Jeroen Krijgsveld[1]; *[1]German Cancer Research Center (DKFZ), Heidelberg, Germany; [2]CeMM 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 Zhu[1]; Shuling Xu[1]; Zicong Wang[1]; Daniel G. Delafield[1]; Michael J. Rigby[1]; Gaoyuan Lu[1]; Ting-Jia Gu[1]; Peng-Kai Liu[1]; Min Ma[1]; Luigi Puglielli[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WOG am 09:10 **Deep Proteome Turnover in human iPSC-derived Neurons**; Ashley Frankenfield[1]; Jiawei Ni[1]; Jamison Shih[1]; Noah Smeriglio[1]; Ling Hao[1]; *[1]George Washington University, Washington, DC*

WOG am 09:30 **Aziridination-Based 2-Aminopyridine Isotopic (AAPI) Tag Enables Lipid Accurate Quantification with Isomer Resolving Power**; Shuli Tang[1]; Syuan-Ting Kuo[1]; Hongyuan Yang[1]; Luchen Wuyang[1]; Jiaxin Feng[1]; Xin Yan[1]; *[1]Texas A&M University, College Station, TX*

WOG am 09:50 **Spatial Neutron-Encoded Stable Isotopic Labeling of Three-Dimensional Multicellular Spheroids**; Arbil Lopez[1]; Nicole C. Beller[1]; Amanda B Hummon[1]; *[1]The 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 Yang[1]; Qing Yu[1]; Shane Lillis Dawson[1]; Joao A. Paulo[1]; Steven P. Gygi[1]; *[1]Harvard 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 Consta[1]; Yiming Qin[2]; *[1]University of Western Ontario, London; [2]University 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 McPartlan[1]; Conner C. Harper[1]; Emeline Hanozin[1]; Evan R. Williams[1]; *[1]University 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 Shepherd[1]; Austin W Green[2]; Kenneth R Newton[2, 3]; Elizabeth S Resendiz[4]; Ruwan T Kurulugama[5]; James S Prell[2]; *[1]University of Oregon, Eugene, OR; [2]University of Oregon, Department of Chemistry and Biochemistry, Eugene, OR; [3]e-MSion, Corvallis, OR; [4]University of California, Irvine, Irvine, CA; [5]Agilent Technologies, Santa Clara, CA*

WOH am 09:50 **Measuring the absolute energy differences between conformers of protonated GlyProGlyGly**; Brandon C. Stevenson[1]; Shannon Raab[2]; David E. Clemmer[2]; Peter B. Armentrout[1]; *[1]University of Utah, Salt Lake City, UT; [2]Indiana 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 Girod[1]; Jean-Valery Guillaubez[1]; Jérôme Lemoine[1]; *[1]University of Lyon, Villeurbanne, France*

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 Jarrold; *Indiana University, Chemistry Department, Bloomington, IN*

WOA pm 02:50 **Benefits of ultra-long transients in Orbitrap based charge-detection mass spectrometry**; Evolène Deslignière[1]; Victor Yin[1]; Amber Rolland[1]; Eduard Ebberink[1]; Arjan Barendregt[1]; Tobias P. Wörner[2]; Konstantin Nagornov[3]; Anton Kozhinov[3]; Kyle L. Fort[2]; Yury O. Tsybin[3]; Alexander A. Makarov[2]; Albert J.R. Heck[1]; *[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. Woerner[2]; Maria Reinhardt-Szyba[2]; Kyle L. Fort[2]; Frank Sobott[1]; Alexander A. Makarov[2]; *[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 Wörner[1]; Hayden A Thurman[2]; Alexander A Makarov[1]; Alexandre A Shvartsburg[2]; *[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. Shaw[1]; Sophie R. Harvey[2]; Chen Du[3]; 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 Harper[1]; Zachary M. Miller[1]; Matthew S. McPartlan[1]; Jacob S. Jordan[1]; Evan R. Williams[1]; *[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 Schär[1]; Marco Tognetti[1]; Roland Bruderer[2]; Lukas Reiter[2]; *[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 Mehta[1]; Kristin Boylan[1]; Ashley J. Petersen[1]; Amy P.N. Skubitz[1]; Pratik D Jagtap[1]; Timothy J Griffin[1]; *[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 Metatla[1]; Kévin Roger[1]; Cerina Chhuon[1]; Anne Jamet[2]; Maria Leite De Moraes[2]; Manuel Chapelle[3]; Pierre-Olivier Schmit[3]; Chiara Guerrera[1]; *[1]Proteomics Platform Necker, Paris, France; [2]INSERM U1151 - CNRS 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 Pannkuk[1]; Evagelia Laiakis[1]; Guy Garty[2]; Brian Ponnaiya[2]; Xuefeng Wu[2]; Igor Shuryak[2]; Shanaz Ghandhi[2]; Sally Amundson[2]; David Brenner[2]; 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 Banarjee[1]; Bradley Olinger[1]; Dimitrios Tsitsipatis[1]; Anjana Ram[1]; Thedoe Nyunt[1]; Ceereena Ubaida-Mohien[1]; Gulzar Daya[1]; Zhongsheng Peng[1]; Myriam Gorospe[1]; Luigi Ferrucci[1]; Keenan Walker[1]; Nathan Basisty[1]; *[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 Broeckling[1]; Richard Beger[2]; Leo L Cheng[3]; Raquel Cumeras[4]; Daniel J Cuthbertson[5]; Surendra Dasari[6]; Clay W Davis[7]; Warwick B Dunn[8]; Anne M Evans[9]; Álvaro Fernández-Ochoa[10]; Kelli D Goodman[9]; Helen Gika[11]; Royston Goodacre[8]; Goncalo J Gouveia[12]; Hsu Ping-Ching[13]; Jennifer A Kriwan[14]; Dritan Kodra[11]; Julia Kuligowski[15]; Lan S Renny[16]; María Eugenia Monge[17]; Jonathan D Mosley[18]; Sindhu Nair[19]; Nichole Reisdorph[20]; Stacy D Sherrod[21]; Georgios Theodoridis[11]; Candice Z Ulmer Holland[22]; Dajana Vuckovic[23]; Bo Zhang[24]; *[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 Zhao[1]; Liang Li[1]; *[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 Mannochio Russo[1]; Ipsita Mohanty[1]; Yasin El Abiead[1]; Joshua V Schweer[1]; Robin Schmid[1]; Simone Zuffa[1]; Wout

Bittremieux[2]; Felipe Vasquez-Castro[1]; Andrew D Patterson[3]; Dionicio Siegel[1]; Lee Hagey[1]; Mingxun Wang[4]; Allegra T Aron[5]; Pieter C Dorrestein[1]; *[1]University of California San Diego, San Diego, CA; [2]University of Antwerp, Antwerpen, Belgium; [3]Pennsylvania State University, State College, University Park, PA 16803; [4]University of California Riverside, Riverside, CA; [5]University 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 Rodriguez[1]; Uri Keshet[1]; Bashar Amer[2]; Sunandini Yelda[3]; Brandon Bills[3]; Tong Shen[1]; Susan Bird[3]; Oliver Fiehn[1]; *[1]University of California Davis, Davis, CA; [2]Thermo Fisher Scientific, San Jose, California; [3]ThermoFisher 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 Swann[1]; Wisenave Arulvasan[1]; Ace Hatch[1]; Julia Greenwood[1]; Dominic Roberts[2]; Billy Boyle[1]; Max Allsworth[1]; *[1]Owlstone Medical, Cambridge, United Kingdom; [2]Thermo Fisher Scientific, Manchester, United Kingdom*

WOC pm 04:10 **Development of a multi-omic approach for microorganism identifications**; Jana M Carpenter[1]; Kingsley Bimpeh[1]; Hannah Hynds[1]; Kelly Hines[1]; *[1]University 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-Patiño[2]; Ryan P Rodgers[1, 2]; Alan G Marshall[1, 2]; *[1]Florida State University, Tallahassee, FL; [2]National 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 Riusech[1]; Lingjun Li[1]; *[1]University of Wisconsin, Madison, WI*

WOD pm 03:10 **Structural Elucidation of Lipopolysaccharides using Field Asymmetric Ion Mobility Spectrometry and Kendrick Mass Defect Plots**; Abanoub Mikhael[1]; Darryl Hardie[1]; Derek Smith[1]; Helena Petrosova[1]; Robert K Ernst[2]; David R Goodlett[1, 3]; *[1]University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; [2]University of Maryland, Baltimore, MD; [3]University 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 Abdullah[1]; Cynthia Sommers[1]; Jason Rodriguez[1]; Deyi Zhang[2]; Darby Kozak[2]; Kui Yang[1]; *[1]US Food and Drug Administration, Saint Louis, MO; [2]US 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 Fu[1]; Tabiwang N. Arrey[2]; Niveda Sundararaman[1]; Eugen Damoc[2]; Yue Xuan[2]; Jennifer E. Van Eyk[1]; *[1]Cedars Sinai Medical Center, Los Angeles, CA; [2]Thermo Fisher Scientific, Bremen, Germany*

WOD pm 04:10 **Polymer Analysis on a High-Resolution Quadrupole-Multi Reflecting Time-of-Flight Mass Spectrometer**; Bryan C. Katzenmeyer[1]; Dale A. Cooper-Shepherd[2]; Martin E. Palmer[3]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters, 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 Amirav[1]; Benny Neumark[1]; Oneg Elkabets[1]; Alex Yakovchuk[1]; *[1]Tel-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 Zheng[1]; Edward Erisman[1]; Tytus D. Mak[1]; Weihua Ji[1]; William E. Wallace[1]; Stephen E. Stein[1]; *[1]NIST, 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]; *[1]Catalan Institute for Water Research (ICRA), Girona, Spain; [2]University of Girona, Girona, Spain; [3]Institute 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 andits application to breath biomarker discovery**; Yuta Matsuoka[1]; Yuki Sugiura[2]; *[1]Kyoto university, Kyoto, Japan; [2]Kyoto University, Kyoto, Japan*

WOE pm 03:50 **Exploring Mosquito Olfactory Preferences with Whole Body Volatilomics**; Stephanie Rankin-Turner[1]; Diego Giraldo[1]; Conor McMeniman[1]; *[1]Johns 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. Rowell[1]; Jacob D. Guthrie[1]; Michael E. Peretich[2]; Gozdem Kilaz[1]; Hilkka I. Kenttämaa[1]; *[1]Purdue University, West Lafayette, IN; [2]Naval Air Warfare Center Aircraft Division, Patuxent River, MD*

WOF pm: Quantitative Proteomics in Systems Biology
General Assembly A
Session Chair: Keriann 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 Gygi[1]; Qing Yu[1]; Xinyue Liu[1]; Mark Keller[2]; Tian Zhang[1]; Steven Shuken[1]; Ernst Schmid[1]; Edward L Huttlin[1]; Devin Schweppe[3]; Alan D Attie[4]; Joao A Paulo[1]; *[1]Harvard Medical School, Boston, MA; [2]University of Wisconsin-Madison, Madison, WI; [3]University of Washington, Seattle, WA; [4]University 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 Hinkle[4]; Christopher Mullen[5]; John EP Syka[5]; Carol V Robinson[1, 2]; *[1]Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom; [2]Department of Chemistry, University of Oxford, Oxford, United Kingdom; [3]School of Chemistry, UNSW Sydney, Sydney,* *Australia; [4]Thermo Fisher Scientific, San Jose, CA; [5]ThermoFisher Scientific, San Jose, CA*

WOF pm 03:10 **A multidimensional proteomic atlas of replicative aging in budding yeast**; Mario Leutert[1]; Joe Armstrong[1]; Anja R Ollodart[1]; Kyle N Hess[1]; Michael Muir[2]; Ricard A Rodriguez-Mias[1]; Matt Kaeberlein[2]; Maitreya Dunham[1]; Judit Villén[1]; *[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 Stecker[1]; Sofia Ibanez-Molero[2]; Tatiana M. Shamorkina[1]; Rosa Viner[3]; Daniel S. Peeper[2]; Maarten A.F.M. Altelaar[1]; *[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 Zeller[1]; Jenny Ho[2]; Amirmansoor Hakimi[3]; Maowei Dou[4]; Ryan Bomgarden[4]; Rosa Viner[3]; Bernd Hagedorn[1]; Ankit Dwivedi[1]; Nicolaie Eugen Damoc[1]; *[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 Kuhn[1]; Natalie Clark[1]; D. R. Mani[1]; Adi Goldstein[2]; Yaara Oren[2]; Steven A Carr[1]; Namrata D Udeshi[1]; *[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.**; Richard Cox[1]; Amanda D. French[1]; Kali M. Melby[1]; Micah Prange[1]; Niri Govind[1]; *[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 Kang[1]; Arup Mondal[1]; Julia R. Bonney[1]; Alberto Perez[1]; Boone M. Prentice[1]; *[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 Schramm[1]; Tomoya Tamadate[2]; Christopher J Hogan[2]; Brian H Clowers[1]; *[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 Edwards[1]; Erin A. Hirtzel[2]; Dallas Freitas[2]; Annesha Sengupta[2]; Joohan Kim[2]; Xin Yan[2]; *[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 Ucur[1]; Oisin J Shiels[1]; Alan T Maccarone[1]; Shane R. Ellis[1, 2]; Stephen J Blanksby[3]; Adam J Trevitt[1]; *[1]University of Wollongong, School of Chemistry, Wollongong, Australia; [2]Illawarra Health and Medical Research Institute, Wollongong, Australia; [3]Central Analytical Research Facility, Institute for Future Environments, Brisbane, Australia*

WOG pm 04:10 **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 Krajewski[1]; Kirsten A Cottrill[2]; Willam A Bragg[1]; Brady R Cunningham[1]; Noelani R Boise[3]; Kristin D Victry[3]; Dana L Woodruff[3]; Karen L Wahl[3]; David S Wunschel[3]; Rudolph C Johnson[1]; Elizabeth I Hamelin[1]; *[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 Bills[1]; Sunandini Yedla[1]; Ed George[1]; Juan Sanchez[1]; Tim Stratton[1]; Ralf Tautenhahn[1]; Vlad Zabrouskov[1]; *[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 Tian[1]; Shaghig Bilamjian[1]; Tarun Anumol[2]; Daniel Cuthbertson[2]; Stéphane Bayen[1]; *[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. Harsha[1]; Danielle E. Verna[2]; Zachary C. Redman[3]; Josh Wesolowski[3]; Angelique Fouche[3]; 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 Dukes[1]; Carrie A McDonough[2]; *[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. Fisher[1]; Ann M. Knolhoff[1]; *[1]FDA Center for Food Safety, College Park, MD*

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. Williams[1]; [1]*University 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 Polack[2]; Manxi Yang[1]; Xiangtang Li[3]; Detlev Belder[2]; Julia Laskin[3]; [1]*Purdue University, West Lafayette, IN;* [2]*Leipzig University, Leipzig, Germany;* [3]*Purdue University, Lafayette, IN*

ThOA am 09:10 **Towards Molecular Digital Twins for Oncology Surgery with Real-Time SpiderMass Mass Spectrometry Imaging**; Nina Ogrinc[1]; Paul Chaillou[1]; Lea Ledoux[1]; Michel Salzet[1]; Isabelle Fournier[1]; [1]*PRISM 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. Tega[2]; Alessandra Sussulini[2]; Xin Yan[3]; Lane A. Baker[3]; [1]*Texas A&M, College Station, TX;* [2]*University of Campinas, Campinas, Brazil;* [3]*Texas A&M Chemistry, College Station, TX*

ThOA am 09:50 **Temperature-Controllable Spark Probe Ionization for Multi-dimensional Mass Spectrometer Analysis**; Ningxi Li[1]; Xinwei Liu[1]; Zhijun Cai[1]; Zongyao Zhang[1]; Jiexun Bu[2]; Simin Cheng[1]; Xiaoxiao Ma[1]; Wenpeng Zhang[1]; Xiaoyu Zhou[1]; Zheng Ouyang[1]; [1]*Tsinghua University, Beijing, China;* [2]*PURSPEC 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 Rorrer[1]; Mitch Wells[1]; Megan Guetzloff[1]; Jane Likens[1]; Nicole Huckaby[1]; Harman Casey[1]; Kevin Rosenbaum[1]; Brandon Reese[1]; Austin Stieglitz[1]; Anthony Eshleman[1]; Luther Collins[1]; Brett Atkinson[1]; [1]*Teledyne 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 Chongsaritsinsuk[1]; Alexandra D. Steigmeyer[1]; Keira E. Mahoney[1]; Mia A. Rosenfeld[2]; Taryn M. Lucas[1]; Deniz Ince[1]; Fiona L. Kearns[2]; Alexandria Battison[1]; Michael J. Ferracane[3]; Rommie E. Amaro[2]; Stacy A. Malaker[1]; [1]*Yale University, New Haven, CT;* [2]*University of California San Diego, San Diego, CA;* [3]*University of Redlands, Redlands, CA*

ThOB am 08:50 **Benefits of dual ion routing multipoles for glycoproteomics**; Nicholas M. Riley[1, 2]; Jingjing Huang[3]; David Bergen[3]; William D. Barshop[3]; John E.P. Syka[3]; Jesse D. Canterbury[3]; Vlad Zabrouskov[3]; Graeme C. McAlister[3]; Christopher Mullen[3]; [1]*Stanford University, Stanford, CA;* [2]*University of Washington, Seattle, WA;* [3]*Thermo 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 Vainauskas[2]; Christopher H. Taron[2]; Jennifer S. Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX;* [2]*New 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]; [1]*IAMS, Academia Sinica, Taipei, Taiwan;* [2]*International Graduate Program of Science and Technology (MST), National Taiwan University, Taipei, Taiwan;* [3]*Molecular Science and Technology (MST), Taiwan International Graduate Program (TIGP), Taipei, Taiwan;* [4]*Department of Chemistry, National Taiwan Normal University, Taipei, Taiwan;* [5]*Department f Chemistry, National Tsing Hua University, Hsinchu, Taiwan;* [6]*Chemical Biology and Molecular Biophysics Program, Taiwan International Graduate Program, Academia Sinica, Taipei, Taiwan;* [7]*Academia 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 Li[2]; Yinlong Zhu[3, 4]; Yingyi Zhao[5]; Feixuan Wu[1]; Zicong Wang[1]; Yu Feng[1]; Hung-Yu Chiang[6]; Cheng Chang[3, 7]; Lingjun Li[1, 8]; [1]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI;* [2]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [3]*State Key Laboratory of Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences (Beijing), Beijing Institute of Lifeomics, Beijing, China;* [4]*Chongqing Key Laboratory on Big Data for Bio Intelligence, Chongqing University of Posts and Telecommunications, Chongqing, China;* [5]*State Key Laboratory of Proteomics, Beijing Proteome Research Center, National Center for Protein Sciences (Beijing), Beijing Institute of Lifeomics,, Beijing, China;* [6]*Biophysics Program, University of Wisconsin–Madison, Madison, WI;* [7]*Research Unit of Proteomics Driven Cancer Precision Medicine, Chinese Academy of Medical Sciences, Beijing, China;* [8]*Department 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 Lu[2]; Fengchao Yu[1]; Guo Ci Teo[1]; Michael R. Shortreed[3]; Alexey I. Nesvizhskii[1]; [1]*University of Michigan, Ann Arbor, MI;* [2]*University of California San Francisco, San Francisco, CA;* [3]*University 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 Wohlgemuth[1]; Fanzhou Kong[1]; Yuanyue Li[1]; Diego Pedrosa[1]; Oliver Fiehn[1]; [1]*UC 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 Acquavia[1]; Carmine Gaeta[2]; Patrizia Iannece[2]; Rosanna Ciriello[1]; Filomena Lelario[1]; Carmen Tesoro[1]; Roberto Rubino[3]; Giuliana Bianco[1]; [1]*Università degli Studi della Basilicata, Dipartimento di Scienze, via dell'Ateneo Lucano 10, 85100, Potenza, Italy;* [2]*Università Degli Studi di Salerno, Dipartimento di Chimica e Biologia, Via Giovanni Paolo II 132,84084, Fisciano (SA), Italy;* [3]*ANFoSC - Via San Leonardo 62/A, 84131, Salerno, Italy*

ThOC am 09:10 **Dual column chromatography improves non-targeted analysis coverage when assessing rhizosphere chemical communication**; Alexandra A Bennett[1]; Çağla Görkem Eroğlu[2]; Teresa Steininger-Mairinger[1]; Markus Puschenreiter[3]; Aurélie Gfeller[2]; Judith Wirth[2]; Stephan Hann[1]; *[1]University of Natural Resources and Life Sciences, Vienna, Department of Chemistry, Institute of Analytical Chemistry, Vienna, Austria; [2]Agroscope, Department of Plant-Production Systems, Herbology in Field Crops Research Group, Nyon, Switzerland; [3]University 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. Sasiene[1]; Erick S. Lebrun[1]; Eric G. Schaller[2]; Phillip M. Mach[1]; Robert M. Taylor[2]; Trevor G. Glaros[1]; Justin T. Baca[2]; Ethan M. McBride[1]; *[1]Los Alamos National Laboratory, Los Alamos, NM; [2]University 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 Rana[1]; Vivek Mishra[2]; Prajval Nakrani[2]; Bhushan Burkul[2]; Rakesh Kumar Sahay[3]; Lakshman Kumar[3]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Clarity Bio Systems India Pvt Ltd, Pune, India; [3]osmania medical college, Hyderabad, India*

ThOC am 10:10 **Molecular network-based optimization of annotations in GC-MS**; Alexander Semenov[1]; Vladimir Boginski[2]; Alexey Melnik[3]; Alexander Aksenov[3]; *[1]University of Florida, Gainesville, FL; [2]University of Central Florida, Orlando, FL; [3]University of Connecticut, Storrs, CT*

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 Keshishian[1]; Michael W. Burgess[1]; Sebastian Vaca[2]; Joseph Allen[1]; Elizabeth D. Lightbody[3]; Irene M. Ghobrial[3]; D. R. Mani[1]; Michael A. Gillette[1, 4]; Matt Willetts[5]; Steven A Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Bruker Scientific, San Jose, CA; [3]Dana Farber Cancer Institute, Boston, MA; [4]Massachusetts General Hospital, Boston, MA; [5]Bruker Scientific, LLC, Billerica, MA*

ThOD am 08:50 **Multiplex-DIA enhances single-cell proteomic depth via a reference channel**; Marvin Thielert[1]; Corazon Ericka Mae Itang[2]; Constantin Ammar[2]; Florian A. Rosenberger[2]; Isabell Bludau[2]; Patricia Skowronek[2]; Maria Wahle[2]; Wen-Feng Zeng[2]; Xie-Xuan Zhou[2]; Andreas-David Brunner[2, 3]; Sabrina Richter[4, 5]; Fabian J Theis[4, 5]; Martin Steger[2, 6]; Matthias Mann[2, 7]; *[1]Max Planck Institute of Biochemistry, Martinsried, Munich, Germany; [2]Max-Planck-Institute for Biochemistry, Martinsried, Germany; [3]Boehringer Ingelheim Pharma, Biberach, Germany; [4]Helmholtz Zentrum München – German Research Center for Environmental Health, Neuherberg, Germany; [5]Technical University of Munich, Freising, Germany; [6]NEOsphere Biotechnologies GmbH, Planegg, Germany; [7]Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark*

ThOD am 09:10 **Rapid single-shot proteomics using narrow window DIA on a novel high-resolution accurate mass (HRAM) platform**; Ana Martinez Del Val[1]; Ulises H. Guzmán[1]; Zilu Ye[1]; Florian Harking[1]; Ole Østergaard[1]; Anna Pashkova[2]; Tabiwang N. Arrey[2]; Hamish Stewart[2]; Yue Xuan[2]; Nicolaie Eugen Damoc[2]; Jesper V. Olsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThOD am 09:30 **A protein turnover atlas across 15 mouse tissues established by DIA and TMT**; Wenxue Li[1]; Ka Yang[2]; Abhijit Dasgupta[2]; Junmin Peng[2]; Yansheng Liu[1]; *[1]Yale Cancer Biology Institute, West Haven, CT; [2]St. 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 Bayne[1]; Yanlong Zhu[2, 3]; Kevin M. Buck[1]; Melissa R. Pergande[2, 3]; Vanessa Morales-Tirado[4]; Yupeng He[5]; Yu Tian[6]; Ying Ge[1, 2, 3]; *[1]Department of Chemistry, University of Wisconsin - Madison, Madison, WI; [2]Department of Cell and Regenerative Biology, University of Wisconsin - Madison, Madison, WI; [3]Human Proteomics Program, University of Wisconsin - Madison, Madison, WI; [4]Discovery Immunology, Pharmacology and Pathology, AbbVie Bioresearch Center, Worcester, MA; [5]Discovery Immunology, Pharmacology and Pathology, AbbVie Inc., North Chicago, IL; [6]DMPK-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 Ai[1]; Aleksandr Stotland[1]; Simion Kreimer[1]; Matthew Ayres[1]; Juliana De Freitas Germano[1]; Chengqun Huang[1]; Tauseef Butt[2]; Suresh Kumar[2]; Roberta Gottlieb[1]; Jennifer Van Eyk[1]; *[1]Cedars-Sinai Medical Center, Los Angeles, CA; [2]Progenra Inc, Malvern, PA*

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. Abikhodr[1]; Stephan Warnke[1]; Ahmed Ben Faleh[1]; Vasyl Yatsyna[1]; Thomas Rizzo[1]; *[1]Ecole 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 Gichuhi[1]; Aidan J. Usher[1]; Kie T. Workman[1]; *[1]Tennessee 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 Bonney[1]; Boone M. Prentice[1]; *[1]University 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 Zima[1]; Jiahao Wan[1]; Mikuláš Vlk[2]; Josef Cvačka[2]; František Tureček[1]; *[1]University of Washington, Seattle, WA; [2]Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic*

ThOE am 09:50 **A universal photosensitizer for isomer-resolved mass spectrometry imaging of lipids using singlet oxygen reaction**; Sara Amer[1]; Daisy M Unishuay Vila[1,2]; Mushfeqa Iqfath[1]; Julia Laskin[1]; *[1]Purdue University, West lafayette, Indiana; [2]University of Pennsylvania, Philadelphia, PA*

ThOE am 10:10 **Characterization of sialylated N-glycopeptide isomers on reversed phase LC-ECD mass spectrometry**; Suya Liu[1]; Zoe Zhang[1]; Pavel Ryumin[1]; Takashi Baba[1]; *[1]AB 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. Huttlin[1]; Julian Mintseris[1]; Roger Vargas[1]; Laura Pontano Vaites[1]; Tyrone Lee[1]; Sanjukta Guha Thakurta[1]; Lana D'Addieco[1]; Fana Gebreab[1]; Emily Hill[1]; Daniel Linnehan[1]; David Vanderwall[1]; Brandon Gassaway[1]; Sherry Liu[1]; Joao A Paulo[1]; Qing Yu[1]; Jose Navarrete-Perea[1]; Josh Pan[2]; David P Nusinow[3]; Tess C Branon[3]; Donald S Kirkpatrick[3]; Ludwig Geistlinger[1]; Robert Gentleman[1]; J. Wade Harper[1]; Steve Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]Broad Institute of MIT and Harvard, Cambridge, MA; [3]Interline 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 McFadden[3]; Bruce E Torbett[4,5]; Stefan G Sarafianos[3,6]; Vicki H Wysocki[1,2]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; [2]Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; [3]Center for ViroSciences and Cure, Laboratory of Biochemical Pharmacology, Department of Pediatrics, Emory University School of Medicine, Atlanta, Georgia; [4]Department of Pediatrics, University of Washington School of Medicine, Seattle, WA; [5]Center for Immunity and Immunotherapies, Seattle Children's Research Institute, Seattle, WA; [6]Children's Healthcare of Atlanta, Atlanta, Georgia*

ThOF am 09:10 **Native Top-Down Mass Spectrometry Probes Membrane Protein Structures and Lipid Binding Sites**; Jessie Le[1]; Pascal Egea[2]; Mark Arbing[2]; Rachel R. Ogorzalek Loo[2]; Joseph A. Loo[2]; *[1]University of California - Los Angeles, Los Angeles, CA; [2]University 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 Hopper[1]; Kleitos Sokratous[1]; Antonio Biasutto[1]; Emma Norgate[1]; James Lloyd[2]; Karolina Gherbi[1]; Idlir Liko[1]; Neil Oldham[2]; *[1]OMass Therapeutics, Oxford, United Kingdom; [2]University of Nottingham, Nottingham, United Kingdom*

ThOF am 09:50 **RAPID ANALYSIS OF PROTEIN-PROTEIN INTERACTIONS USING A NOVEL HIGH-RESOLUTION ACCURATE MASS PLATFORM**; Lia Serrano[1]; Danielle Swaney[2,3,4,5]; Tabiwang N. Arrey[6]; Trenton M. Peters-Clarke[1]; Noah M Lancaster[1]; Anna Pashkova[6]; Evgenia Shishkova[1]; Michael S. Westphall[1]; Christian Hock[6]; Nicolaie Eugen Damoc[6]; Vlad Zabrouskov[6]; Joshua J. Coon[1,7]; *[1]University of Wisconsin-Madison, Madison, WI; [2]QBI COVID-19 Research Group (QCRG), San Francisco, CA; [3]Quantitative Biosciences Institute (QBI), University of California San Francisco, San Francisco, CA; [4]J. David Gladstone Institutes, San Francisco, CA; [5]Department of Cellular and Molecular Pharmacology, University of California San Francisco, San Francisco, CA; [6]Thermo Fisher Scientific, Bremen, Germany; [7]Morgridge 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 Habeck[1]; Kyle A. Brown[2]; Benjamin Des Soye[3]; Carter Lantz[4]; Mowei Zhou[5]; Novera Alam[6]; Md Amin Hossain[6]; Wonhyeuk Jung[4]; James E. Keener[7]; Michael Volny[8]; Jesse W. Wilson[5]; Yujia Ying[9]; Jeffrey N. Agar[6]; Paul O. Danis[10]; Ying Ge[2]; Neil L. Kelleher[3]; Huilin Li[9]; Joseph A. Loo[4]; Michael T. Marty[7]; Ljiljana Paša-Tolić[5]; Wendy Sandoval[8]; Frederik Lermyte[1]; *[1]Technical University of Darmstadt, Darmstadt, Germany; [2]University of Wisconsin-Madison, Madison, WI; [3]Northwestern University, Evanston, IL; [4]University of California, Los Angeles, Los Angeles, CA; [5]Pacific Northwest National Laboratory, Richland, WA; [6]Northeastern University, Boston, MA; [7]University of Arizona, Tucson, AZ; [8]Genentech Inc, South San Francisco, CA; [9]Sun Yat-sen University, Guangzhou, China; [10]Consortium 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 Anzola[5]; Evan R. Hutchison[3]; Eugenio I. Vivas[3]; Robert L. Kerby[3]; Nsoua H. Diaba[6]; Camil Gosmanov[6]; Alejandro Reyes Muñoz[5]; Federico E. Rey[3]; Laura-Isobel McCall[2,6,7]; *[1]University of Oklahoma, Department of Anthropology, Norman, OK; [2]University of Oklahoma, Laboratories of Molecular Anthropology and Microbiome Research, Norman, OK; [3]University of Wisconsin-Madison, Department of Bacteriology, Madison, WI; [4]Northwest A&F University, College of Food Science and Engineering, Xianyang, China; [5]Universisdad de los Andes, Departamento de Ciencias Biológicas, Bogotá, Colombia; [6]University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; [7]University 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 Bishop[1]; Ayush Mandwal[1]; Mehdi Mohammadi[1]; Thomas Rydzak[1]; Ryan A Groves[1]; Mildred Castellanos[1]; George Chaconas[1]; Joern Davidsen[1]; Ian A Lewis[1]; *[1]University 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 Dumas[1]; Olivier Pible[1]; Guylaine Miotello[1]; Kristina Marx[2]; Pierre-Olivier Schmit[2,3]; Jean Armengaud[1]; *[1]CEA-Marcoule - Laboratory «Innovative technologies for Detection and Diagnostics», Bagnols-sur-Cèze, France; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [3]Bruker France S.A., Wissembourg, France*

ThOG am 09:30 **On-chip multi-modal imaging of soil biogeochemical processes using Synthetic Soil Habitats**; Arunima Bhattacharjee[1]; Jocelyn Richardson[2]; Dušan Veličković[1]; Gregory Vandergrift[1]; Christopher Anderton[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Stanford University, Palo Alto, CA*

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 Migas[3]; Madeline E Colley[4, 5]; Martin Dufresne[2, 5]; Jeffrey A Freiberg[6]; Valeria M Reyes Ruiz[6]; Andy Weiss[6]; Katerina V Djambazova[2, 7]; Katherine N GIbson-Corley[6]; Raf Van De Plas[2, 3, 5]; Eric P Skaar[6]; 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 Lakshmanan[1]; Andrew Rodriguez[1]; Phil Olsen[1]; Dennis Rhodes[1]; Claus Rentel[1]; *[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 Welbourne[1]; Caroline Evans[1]; Christina Vanhinsbergh[1]; Mark Dickman[1]; *[1]University of Sheffield, Sheffield, United Kingdom*

ThOH am 09:10 **LC-HRMS-based Multi-Attribute Method for Oligonucleotides (MAMO)**; Kui Yang[1]; A M Abdullah[1]; Md Rabiul Islam[1]; Nnenna E Dieke[1]; Cynthia Sommers[1]; Jason Rodriguez[1]; Deyi Zhang[2]; Darby Kozak[2]; David Keire[1]; *[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 Jakes[1]; Maikel Gaitkoski[1, 2]; Felipe Guapo[1]; Silvia Millan Martin[1]; Sara Carillo[1]; 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 Brundridge[1]; Jonathan Dickerhoff[1]; Danzhou Yang[1]; Scott A McLuckey[1]; *[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 Ivanov[1]; John J Thomas[2]; Dani M Stoltzfus[2]; Igor A Kaltashov[1]; *[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 Webber[1]; Siqi Huang[1]; Thy Truong[1]; Xiaofeng Xie[1]; Ryan Kelly[1]; *[1]Brigham 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 Chen[1]; Chin-Ming Kuo[1]; Fung-Yu Chen[1]; *[1]National Cheng Kung University, Tainan, Taiwan*

ThOA pm 03:10 **Exploring Charge Detection Mass Spectrometry on Liquid Chromatography Time Scales**; Lisa Strasser[1]; Florian Fuessl[1]; Tomos E. Morgan[1]; Felipe Guapo[1]; Sara Carillo[1]; Jonathan Bones[1,2]; *[1]NIBRT, Dublin, Ireland; [2]School 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 Mellors[1]; Youwei Chen[2]; Timothy McMahon[2]; Matthew W Foster[2]; *[1]908 Devices Inc, Carrboro, NC; [2]Duke 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 Debord[1]; Liulin Deng[1]; Brian Adamson[2]; Alan McKenzie-Coe[1]; Kyle L. Fort[3]; Tobias Woerner[3]; Oliver M Bernhardt[4]; Roland Bruderer[4]; Tejas Gandhi[4]; Lukas Reiter[4]; Eloy R Wouters[2]; Jean-Jacques Dunyach[2]; Alexander Makarov[3]; *[1]MOBILion Systems, Chadds Ford, PA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [4]Biognosys AG, Schlieren, Switzerland*

ThOA pm 04:10 **Rapid and accurate quantitation of therapeutic drugs by coupling capillary electrophoresis with miniature mass spectrometry system**; Xiao Chen[1]; Junhan Wu[1]; Yikun Liu[1]; Wenpeng Zhang[1]; Zheng Ouyang[1]; *[1]Tsinghua 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 Liu[1]; Yuetian Yan[1]; Shunhai Wang[1]; Ning Li[1]; *[1]Regeneron 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 Powers[1]; Nicole Azer[1]; Aron Gyorgypal[2]; Erica Berilla[1]; Casey Kohnhorst[1]; *[1]FDA, Silver Spring, MD; [2]Rutgers 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-Vega[1]; Hayden Fisher[2]; Isabel Elliott[2]; Mark S Cragg[2]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]University 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**; Benqian Wei[1]; Carter Lantz[1]; Rachel R. Ogorzalek Loo[1]; Iain D. G. Campuzano[2]; Joseph A. Loo[1]; *[1]UCLA, Los Angeles, CA; [2]Amgen, Thousand Oaks, CA*

ThOB pm 03:50 **Antibody structural dynamics investigated by covalent labelling and structure-sensitive fragmentation**; Melissa Ann Coxhead[1]; Dale A. Cooper-Shepherd[2]; Romina Hofele[3]; Paul Devine[4]; Nicholas J. Bond[4]; Frank Sobott[1]; *[1]University of Leeds, Leeds, United Kingdom; [2]Waters Corporation, Stamford Ave, Altrincham Road, Wilmslow, United Kingdom; [3]Analytical Sciences, BioPharmaceutical Development, BioPharmaceuticals R&D, AstraZeneca, Gaithersburg, Maryland; [4]Analytical 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 Bittner[1]; Felix Kuhne[2]; Dietmar Reusch[2]; Renato Zenobi[1]; *[1]ETH Zurich, Zurich, Switzerland; [2]Roche 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 Lefèvre[1]; Emmanuelle Claude[2]; Sylvie Bodard[1]; Sylvie Chalon[1]; Julie Busson[1]; Johnny Vercouillie[1]; Freddy Drouyé[3]; Laurent Galineau[1]; Patrick Emond[1,4]; *[1]University Tours, INSERM, iBrain, UMR 1253, Tours, France; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters Corporation, Guyancourt, France; [4]CHRU 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 Balbisi[1,3]; Christopher Kremslehner[2,4]; Sandra Forestier[2,5]; Gaelle Gendronneau[2,5]; Florian Gruber[2,4]; Martina Marchetti-Deschmann[1,2]; *[1]TU Wien, Vienna, Austria; [2]Christian Doppler Laboratory for Multimodal Imaging of Aging and Senescence - SKINMAGINE, Vienna, Austria; [3]MS Proteomics Research Group, Research Centre for Natural Sciences, Budapest, Hungary; [4]Medical University of Vienna, Department of Dermatology, Vienna, Austria; [5]Chanel 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 Veličković[1]; Jeffrey Hodgin[2]; Theodore Alexandrov[3]; Kumar Sharma[4]; Christopher Anderton[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of Michigan Ann-Arbor, Ann Arbor, MI; [3]EMBL, Heidelberg, Germany; [4]University 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 Redureau[1]; John Dunbar[2]; Antoine Fort[3]; Virginie Bertrand[1]; Raphaël La Rocca[1]; Christopher Kune[1]; Sophie Rappe[1]; Ronan Sulpice[3]; Edwin De Pauw[1]; Michel Dugon[2]; Loic Quinton[1]; *[1]MS-Lab, MOLSys Research Unit,* *University of Liège, Liège, Belgium; [2]Venom Systems Lab - School of Natural Sciences - University of Galway, Galway, Ireland; [3]Plant 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 Jones[1]; Dustyn Barnette[1]; Laura Schnackenberg[1]; Richard Beger[1]; Andrew Shen[1]; Timothy Flanigan[1]; [1]*FDA/NCTR, Jefferson, AR*

ThOC pm 04:10 **Single-cell lipidomics enabled by high-throughput mass spectrometry imaging at subcellular resolution**; Hua Zhang[1]; Yuan Liu[1]; Xudong Shi[2]; Penghsuan Huang[3]; Haiyan Lu[1]; Andrew J. Schneider[4, 5]; Luigi Puglielli[4, 5]; Nathan V. Welham[2]; Lingjun Li[1, 3]; [1]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of Surgery, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WISCONSIN; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [4]Department of Medicine, University of Wisconsin-Madison, Madison, WISCONSIN; [5]Waisman 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 Bataineh[1]; Lauren Schultz[1]; Benjamin J. Bythell[2]; [1]*Ohio Universty, Athens, OH; [2]Ohio University, Athens, OH*

ThOD pm 02:50 **Taming Conformational Heterogeneity of N-Methylated Macrocyclic Peptides on an Ion Race Track**; Thanh D Do[1]; Hernando J. Olivos[2]; Miranda N. Limbach[1]; Damilola S. Oluwatoba[1]; Jonathan K. Martens[3]; Jos Oomens[3]; [1]*University of Tennessee, Knoxville, Knoxville, TN; [2]Waters Corporation, Milford, MA; [3]HFML 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 Pedrete[1]; Tyler C Cropley[1]; Fanny C Liu[1]; Jusung Lee[1]; Christian Bleiholder[1]; [1]*Florida State University, Tallahassee, FL*

ThOD pm 03:30 **Simulations of Surface-Induced Dissociation Mass Spectrometry of a Protein Dimer Essential for Hearing**; Zachary D Smith[1]; Yu-Fu Lin[1]; Dalton Snyder[1, 2]; Vicki H Wysocki[1]; Marcos Sotomayor[1]; [1]*Ohio State University, Columbus, OH; [2]Teledyne FLIR, West Lafayette, IN*

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

ThOD pm 04:10 **Coulomb explosion molecular imaging: direct characterization of complex structures through multivariate analysis**; Michael Burt[1]; Louis Minion[1, 2]; James Somper[1]; [1]*University of Oxford, Oxford, United Kingdom; [2]Imperial 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-Nitrophloroglucinol as an Effective Matrix for Quantitative MALDI MS and Imaging of Fungicide Pyrimethanil in Strawberries**; Heather McDonald[1]; Qi Li[2]; Md Ashaduzzaman[2]; Chao Zhao[2]; Shanlin Pan[2]; Gregory J. Szulczewski[2]; Qiaoli Liang[2]; [1]*University of West Alabama, Livingston, AL; [2]University 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. Forbes[1]; John Pettibone[1]; Eric Windsor[1]; Diana L. Ortiz-Montalvo[1]; Abigail P. Lindstrom[1]; Joseph M. Conny[1]; Robert A. Fletcher[1]; [1]*National 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 Dutt[1]; Adriana Arigò[1]; Giorgio Famiglini[1]; Pierangela Palma[1, 2]; Achille Cappiello[1, 2]; [1]*UNIVERSITY OF URBINO CARLO BO, URBINO, Italy; [2]Vancouver Island University, Nanaimo, BC*

ThOE pm 03:30 **Odor profiling and SIFT-MS analysis reveal relationships for perceived odor duringwastewater treatment**; Michael A McGinley[1]; Olivia Rice[1]; Leslie P. Silva[2]; [1]*St. Croix Sensory, Inc., Stillwater, MN; [2]Syft Technologies, Los Angeles, CA*

ThOE pm 03:50 **Resolving halogenated water disinfection by-products (DBPs) isomers of Bisphenol A with ion mobility - mass spectrometry**; Mauricius Marques Dos Santos[1]; Caixia Li[1]; Shenglan Jia[1]; Shane A Snyder[1]; [1]*Nanyang 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 Vetter[1]; Steffen Bräkling[1]; Sonja Klee[1]; [1]*TOFWERK, 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 Paramo[1]; Dawn Dufield[2]; Rathna Veeramachaneni[2]; Emily Parkhurst[2]; Christopher Harp[1]; Akshaya Ramesh[1]; W. Rodney Mathews[1]; Veronica Anania[1]; [1]*Genentech, South San Francisco, CA; [2]KCAS, Olathe, KS*

ThOF pm 02:50 **Quantitation and Structural Elucidation of Intact Brain Sphingolipids with nanoflow HPLC-MS/MS**; Ryan L Schindler[1]; Jennyfer Tena[1]; Carlito B. Lebrilla[1]; [1]*UC 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 Deshpande[1]; Mandy Bowman[1]; Bashar Amer[1]; Thomas Moehring[2]; Susan Bird[1]; [1]*Thermo Fisher Scientific, San Jose, California; [2]Thermo Fisher Scientific, Bremen, Germany*

ThOF pm 03:30 **Connecting altered branched fatty acid distributions with membrane fluidity in daptomycin-resistant Staphylococcus aureus**; Christian D Freeman[1]; Craig Gatto[2]; Brian J Wilkinson[2]; Vineet K Singh[3]; Kelly M Hines[1]; [1]*University of Georgia, Athens, GA; [2]Illinois state* *university, Normal, IL; [3]A.T. Still Univeristy, Kirksville, MO*

ThOF pm 03:50 **Structural Characterization of Phosphatidylcholine Isomers Using Collisional Induced Dissociation/Electron Induced Dissociation (CID/EID) in Imaging Mass Spectrometry**; Tingting Yan[1]; Zhongling Liang[1]; Boone M. Prentice[1]; *[1]University of Florida, Gainesville, FL*

ThOF pm 04:10 **Investigating the lipidome of small extracellular vesicles**; Adriana Zardini Buzatto[1]; Liang Li[1, 2]; *[1]The Metabolomics Innovation Centre (TMIC), Edmonton, AB; [2]University 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 Krupicka[1]; Aleksandra Popowich[2]; Katell Bathany[1]; Stéphane Claverol[3]; Julie Arslanoglu[2]; Caroline Tokarski[1]; *[1]Institute of Chemistry and Biology of Membrane and NanoObjects (CBMN), CNRS UMR 5248 University of Bordeaux, Bordeaux, France; [2]Department of Scientific Research, The Metropolitan Museum of Art, New York City, NY; [3]Proteome 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 Mulder[1]; Courtney A Cruse[1]; Mark L Miller[2]; *[1]ORISE Visiting Scientist Program - FBI, Quantico, VA; [2]Federal 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 Girard[1]; Patrick Knight[2]; Gerard Hopfgartner[1]; *[1]University of Geneva, Geneva 4, Switzerland; [2]Shimadzu 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. Bondzie[2]; Adewale A. Adehinmoye[2]; Brian T. Molnar[3]; Patrick W. Fedick[3]; *[1]Illinois State University, Normal, IL; [2]Illinois state university, Normal, IL; [3]Naval 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 Erisman[1]; Anthony Kearsley[1]; Yuxue Liang[1]; Edward Sisco[1]; William E. Wallace[1]; *[1]NIST, 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 Rochon[2]; Serge Auger[2]; Jean Lacoursière[2]; Pierre Picard[2]; *[1]Phytronix Technologies, Quebec City, QC; [2]Phytronix Technologies Inc., Quebec, 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 Keshet[1]; Jeremiah D Wells[1]; Oliver Fiehn[1]; *[1]West Coast Metabolomics Center, University of California, DAVIS, CA*

ThOH pm 02:50 **Scalable analysis of untargeted LC-HRMS data by means of SQL database archiving**; Marie Mardal[1, 2]; Brian Schou Rasmussen[2]; Kristian Linnet[2]; Christian Brinch Mollerup[2]; *[1]Department of Pharmacy, the Arctic University of Northern Norway, Tromsø, Norway; [2]Department 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 Vitek[1]; *[1]Northeastern University, Boston, MA*

ThOH pm 03:30 **Molecular networking for the 21st century**; Christoph A. Krettler[1]; John T. Prince[1]; Daniel G. C. Treen[1]; David Healey[1]; Joe Rokicki[1]; *[1]Enveda 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 Simonoff[1]; Yongdong Wang[1]; *[1]Cerno Bioscience, Las Vegas, NV*

ThOH pm 04:10 **Boosting workflow efficiency and productivity with instrument intelligence and smart automation**; Emma E. Rennie[1]; Huy Bui[1]; Patrick Batoon[1]; Christian Klein[1]; James S. Pyke[1]; Li Sun[1]; Haopeng Wang[1]; George Yefchak[1]; *[1]Agilent Technologies, Inc., Santa Clara, 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

Oligonucleaotides 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) paradyms 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 challeanges and solutions. It will start with each panelist giving a 5 min talk overview of their biggest challeange 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 Unv) - sample intergration 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.

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.

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 reenforce 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. I(n 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.

TUESDAY WORKSHOPS, 5:45 – 7:00 PM

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

(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 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 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, deformulating 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.

WEDNESDAY WORKSHOPS, 5:45 – 7:00 PM

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 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 Rüger
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 APLI 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-base 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 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). The 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 Faull

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
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Fundamentals: Ion Molecule, Ion/Ion,
    Ion/Electron Interactions.................................231-248
Fundamentals: Native MS 249-268
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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
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Lipids: General...439-466
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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 I702-721
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 Multari[1]; Michelle F Whitford[1]; Ronika K Power[1]; Paul A Haynes[1]; [1]*Macquarie 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-Sanchez[1]; Maria Serrano Ruber[1]; Anna M. Davies-Barret[1]; Donald J. L. Jones[1]; Sarah A. Inskip[1]; [1]*University 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 Koenig[1]; Palesa Petunia Madupe[1]; Ioannis Patramanis[1]; Patrick L. Rüther[1]; Nomawethu Hlazo[2]; Meaghan Mackie[1, 3]; Lauren Schroeder[4]; Alberto John Taurozzi[1]; Clément Zanolli[5]; Fernando Racimo[1]; Jesper Velgaard Olsen[1]; Rebecca Rogers Ackermann[2]; Enrico Cappellini[1]; [1]*University of Copenhagen, Copenhagen, Denmark;* [2]*University of Cape Town, Cape Town, South Africa;* [3]*University College Dublin, Belfield, Ireland;* [4]*University of Toronto, Toronto, ON;* [5]*Université 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-Deschmann[1]; [1]*TU Wien, Vienna, Austria;* [2]*Academy of Fine Arts Vienna, Vienna, Austria*

MP 005 **Insights into patterns and pathways of protein degradation: A case study with β-lactoglobulin**; Bharath Nair[1]; Meaghan Mackie[2]; Tina Ravnsborg[3]; Samantha Presslee[4]; Kirsty Penkman[4]; Jesper Velgaard Olsen[1]; Ole Jensen[3]; Carsten Wiuf[1]; Matthew Collins[1, 5]; [1]*University of Copenhagen, Copenhagen, Denmark;* [2]*University College Dublin, Belfield, Ireland;* [3]*University of Southern Denmark, Odense, Denmark;* [4]*University of York, Helsington, United Kingdom;* [5]*University 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**; Ilaria Serafini[1, 2]; Gabriele Favero[1]; Roberta Curini[1]; Gwénaëlle M. Kavich[2]; Timothy P. Cleland[2]; Caroline Solazzo[2]; [1]*Sapienza University of Rome, Rome, Italy;* [2]*Smithsonian Museum Conservation Institute, Suitland, MD*

MP 007 **Chromatography-free analysis of pigments by high resolution mass spectrometry with direct sample introduction**; Sam Putnam[1]; Rachel Lackner[2]; William L. Fatigante[1]; Nobuko Shibayama[2]; Maria Goretti Mieites Alonso[2]; [1]*Bruker Scientific, LLC, Billerica, MA;* [2]*The 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. Gould[1]; Rocio Elejalde Cadena[2]; Alan Friedman[3]; Abel Moreno[2]; Troy D. Wood[1]; [1]*Department of Chemistry, University at Buffalo, Buffalo, NY;* [2]*Instituto de Química, Universidad Nacional Autońoma de Mex́ico, Ciudad de México, Mexico;* [3]*Department 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 Hubbard[1]; Steven Robinson[2]; Ardern Hulme-Beaman[3]; Martin Munt[4]; Krzysztof Pawlak[2]; Steve Taylor[1]; [1]*Department of Electrical Engineering & Electronics, University of Liverpool, Liverpool, United Kingdom;* [2]*Materials Innovation Factory, University of Liverpool, Liverpool, United Kingdom;* [3]*University of Liverpool, Liverpool, United Kingdom;* [4]*Dinosaur 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 Huang[3]; Jun

Zhao[3, 4]; Siqi Liu[5]; *[1]BGI, Shenzhen, China; [2]College of Life Sciences, University of Chinese Academy of Sciences, Beijing, China; [3]Shenzhen Eye Institute, Shenzhen Eye Hospital, Jinan University, Shenzhen, China; [4]Department 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; [5]BGI, Shenzhen, China*

MP 011 **Direct measurement of Plasma Phosphatidylinositols and Polyphosphoinositides in Lung Cancer Patients Using UHPLC/MS/MS**; Hai Bui[1]; Kenneth D. Roth[1]; *[1]Eli Lilly and Company, Indianapolis, IN*

MP 012 **Structural proteomic profiling of cerebrospinal fluids to reveal novel conformational biomarkers for Alzheimer's disease**; Bin Wang[1]; Xiaofang Zhong[1]; Lauren Fields[1]; Haiyan Lu[1]; Zexin Zhu[1]; Lingjun Li[1]; *[1]UW-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 Liu[1]; Kun Qian[2]; *[1]Shanghai Jiao Tong University, Shanghai, China; [2]Shanghai Jiao Tong University, Shanghai, China*

MP 015 **Proteomics Analysis of Rheumatoid Arthritis Patients' sera Identifies Multi-Biomarker for Predicting Inflximab Response**; Ara Cho[1]; Jinsung Ahn[1]; Andrew Kim[1]; Eugene C. Yi[1]; *[1]Department 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 Wu[1]; Kun Qian[2]; *[1]Med-X Research Institution, SJTU, Shanghai, China; [2]Shanghai Jiao Tong University, Shanghai, China*

MP 017 **Metabolomic Profiling of Cancer Biomarkers from Methanol Extracts from Pathology Specimens using LC-MS/MS**; Alexandra M. Izydorczak[1]; Wilfrido D. Mojica[1]; Troy D. Wood[1]; *[1]SUNY at Buffalo, Buffalo, NY*

MP 018 **Contribution of the microbiome to a metabolomic signature predictive of risk for pancreatic cancer**; Johannes Fahrmann[1]; Ehsan Irajizad[2]; Jody Vykoukal[2]; Ranran Wu[2]; Jennifer B Dennison[2]; James P Long[2]; Anirban Maitra[2]; Kim-Anh Do[2]; Samir Hanash[2]; *[1]University of Texas, MD Anderson, Houston, TX; [2]UTMDACC, 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 Pu[1]; Qingqing Shen[1]; Chao Xue[1]; Timothy Sikorski[2]; Thomas Angel[2]; Zhuo Chen[2]; John T Mehl[2]; Huaping Tang[2]; Jun Qu[1, 3]; *[1]University at Buffalo, Buffalo, NY; [2]GSK, Collegeville, PA; [3]New 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 Hronowski[1]; Rongfang Gu[1]; Kayla Soucey[1]; Benbo Gao[1]; Zhaohui Shao[1]; Ru Wei[1]; *[1]Biogen, Cambridge, MA*

MP 021 **Biomarker discovery pipeline with chemical isotope labeling LC-MS method**; Wayne Cheng[1]; Rui Qin[1]; Shuang Zhao[1]; Liang Li[1, 2]; *[1]The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta; [2]University of Alberta, Edmonton, AB*

MP 022 **Depleted or non-depleted serum, establishing a best practice approach for monitoring peptide biomarkers using DIA methodologies**; Alison Porter[1]; Abigail Burrows Franco[1]; Cecily R Wood[1]; Scott M Peterman[2]; Scott D Stanley[1]; *[1]University of Kentucky, Lexington, KY; [2]Thermo 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 Shevchenko[1]; Anastasiya Ushenkina[1]; Jonas Bergquist[1, 2]; *[1]Department of Chemistry - Biomedical Center, Analytical Chemistry and Neurochemistry, Uppsala University, Uppsala, Sweden; [2]The 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 Chen[1]; Kuen-Tyng Lin[1]; Yi-Jing Hsiao[2]; Gee-Chen Chang[3]; Jin-Shing Chen[4]; Sung-Liang Yu[2]; Yu-Ju Chen[1]; *[1]Institute of Chemistry, Academia Sinica, Taipei, Taiwan; [2]Department of Clinical Laboratory Sciences and Medical Biotechnology, College of Medicine, National Taiwan University, Taipei, Taiwan; [3]Institute of Medicine of Chung Shan Medical University, Taichung City, Taiwan; [4]Department 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 Postovit[1]; Gilles A Lajoie[2]; *[1]Queen's University, Kingston, ON; [2]Western 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-Bullón[1]; Javier Martin-González[1]; Gloria Muñoz-Fernández[1]; Alberto Jiménez[1]; Jose Luis Revuelta Doval[1]; *[1]University 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 Lucas[1]; Cameron Hill[1]; Elisabeth Karsten[1]; Dana Pascovici[2]; Rosalee McMahon[1]; Ben Herbert[1]; *[1]Sangui Bio, Sydney, Australia; [2]Insight 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 Williams[1]; Mehari Weldemariam[1]; Maureen A. Kane[1]; *[1]University 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 Brunner[1]; Anouk Oldenburger[1]; Larissa Pfisterer[1]; Daniel Veyel[1]; Eva Griesser[1]; Wolfgang Rist[1]; Patrycja Schlingeloff[2]; Julian Schmidberger[2]; Mark Haenle[2]; Wolfgang Kratzer[2]; Heike Neubauer[1]; Markus Werner[1]; Tom Bretschneider[1]; *[1]Boehringer Ingelheim Pharma, Biberach, Germany; [2]Department 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 Muhammednazaar[1]; Anne M Roberts[1]; Ankit Jain[1]; Malcolm Horne[2]; Stephan Klatt[3]; Blaine Roberts[1]; *[1]Emory School of Medicine, Emory University, Atlanta, GA; [2]CSIRO Health and Biosecurity, Herston, Australia; [3]Institue for Vascular Signaling, University of Frankfurt-Goethe University, Germany*

MP 031 **Unbiased Biomarker Discovery for IBD Target Validation and Patient Stratification**; Mostafa J Khan[1]; Faizan Zubair[1]; Chris Deboever[1]; Paul Harris[1]; *[1]Takeda 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 Zhang[1]; Xi Gao[1, 2]; San A[1]; Sang Hua[1]; Wangmu Danzeng[1]; Jin Zi[1]; Siqi Liu[1, 2]; *[1]Beijing Genomics Institute, shenzhen, China; [2]College of Life Sciences, University of Chinese Academy of Sciences, Beijing, China*

MP 033 **Development of proteomic biomarker panel for Cervical Cancer from Indian population**; Amrita Mukherjee[1]; Sanjeeva Srivastava[1]; *[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) Zeng[1]; Hao Qian[1]; Ruby Karimjee[1]; Joon-Yong Lee[1]; Mark Marispini[1]; Jessica Chan[1]; Megan Mora[1]; Benjamin Ta[1]; Ehdieh Khaledian[1]; Chi-Hung Lin[1]; Robert Zawada[1]; Philip Ma[1]; Bruce Wilcox[1]; *[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 Bedillion[1]; Michael Tiemeyer[1]; Franklin E. Leach III[1]; *[1]University of Georgia, Athens, GA*

MP 036 **Quantitative reagent-free bioanalysis of proteins in humanized mouse models: Enrichment and Normalization Strategies**; Jingjing Deng[1]; Eugene Ciccimaro[1]; Petia Shipkova[1]; *[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 Li[1]; Shan Huang[1, 2]; Si Ying Lim[1]; Sock Hwee Tan[1]; Mark Chan[1]; Wuzhong Ni[2]; *[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 Sowle[1]; Tiffany H Seyler[1]; Madeline L Weaver[1]; Lanqing Wang[1]; *[1]CDC, Atlanta, Georgia*

MP 039 **Deep Proteomic Profiling of the Serum Proteome Across the Murine Lifespan**; Amit K Dey[1]; Simonetta Camandola[1]; Nathan L Price[1]; Slam Investigators[1]; Rafael de Cabo[1]; Nathan Basisty[1]; *[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. Nguyen[1]; Jonathan Bui[1]; Zachary Dwight[1]; Jesse G. Meyer[2]; Austin L. Seal[3]; Annie Moradian[1]; Stephen A. Whelan[1]; Mitra Mastali[2]; Sarah J. Parker[2]; David M. Herrington[3]; Susan Mockus[1]; Jennifer E. Van Eyk[2]; *[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 Magomedova[1]; Sophie R Pan[1]; Julia Izhakova[1]; Monica Ortiz[1]; Guy A Higgins[2]; Leo B Silenieks[2]; Ines De Lannoy[1]; *[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**; Maggy Lepine[1]; 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 Hou[1]; Zhu Xiaodong[1]; Bian Alicia[1]; Perry Fan[1]; Andrew Cunningham[1]; *[1]Worldwide Clinical Trials, Austin, TX*

MP 044 **Exploring protein expression across multiple experiments using Mass Dynamics**; Anna Quaglieri[1]; Aaron Triantafyllidis[1]; Bradley Green[1]; Mark Rocco Condina[1]; Paula Burton Ngov[1]; Giuseppe Infusini[1]; Andrew Ian Webb[1, 2, 3]; *[1]Mass Dynamics, Melbourne, Australia; [2]The Walter and Eliza Hall Insitute, 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 Yuan[1]; Kumar Shah[1]; Guoyan Xu[1]; 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 Nilsson[1]; Johan Gobom[1]; Gunnar Brinkmalm[1]; Henrik Zetterberg[1, 2, 3, 4]; Kaj Blennow[1]; Ann Brinkmalm[1]; *[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 Qiu[1]; Thomas Walker[2]; Claudia Gaither[3, 4]; Robert Popp[3]; Christoph H. Borchers[5]; John Sausen[6]; *[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 Rojsajjakul[1]; Clementina Mesaros[1]; Ian Alexander Blair[1]; *[1]University of Pennsylvania, Perelman School of Medicine, Philadelphia, PA*

MP 050 **Comparison of Some Derivatives for the Quantative Analysis of Short-Chain Fatty Acids (SCFA) by LC/MS/MS**; Anna M. Caldwell[1]; John M. Halket[1]; Ana Rodriguez-Mateos[1]; *[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 Wu[1]; Guannan Li[1]; Patrick Batoon[1]; *[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 statusin cultured cells by HPLC-MS/MS**; Jiandong Wu[1]; Anna Chernatynskaya[1]; Annalise Pfaff[1]; Huari Kou[1]; Nan Cen[1]; Nuran Ercal[1]; Honglan Shi[1]; Hu Yang[1]; *[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 applicated to clinical assay**; Thibaut Duval[1]; Aziz Kinani[2]; Laura Akbal[1]; Guillaume Chaplain[2]; Olivier Deschamps[3]; *[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 Bruderer[1]; Dominic Hoch[2]; Luca Raess[1]; Marco Tognetti[1]; Claudia Moresi[1]; Yuehan Feng[1]; Lukas Reiter[1]; *[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 Coppens[1]; Jerome Vialaret[2]; Sylvain Lehmann[2]; Christophe Hirtz[2]; Christopher Hopley[1];

[1]National Measurement Laboratory, LGC, Teddington, United Kingdom; [2]Plateforme de Protéomique Clinique (PPC) Univ Montpellier, CHU Montpellier, INM INSERM, Hôpital St Eloi, IRMB, Montpellier, France

MP 057 **Nanoparticles as alternative affinity reagents for developing targeted mass spectrometric assays of low-abundance biomarkers**; Shane S Kelly[1]; Tai-Tu Lin[1]; Matthew J Gaffrey[1]; Wei-Jun Qian[1]; *[1]Pacific 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 Ranathunge[1]; Sagar S Patel[1]; Lubna Pinky[1, 2]; Vanessa L Correll[1]; Shimin Chen[1]; O. John Semmes[1]; Robert K Armstrong[1]; C. Donald Combs[1]; Julius O Nyalwidhe[1]; *[1]Eastern Virginia Medical School, Norfolk, VA; [2]Meharry Medical College, Nashville, TN*

MP 059 **Quantitation of Gal-1P by LC-MS/MS to evaluate GALT activity after AAV Treatment**; Allison N Schorzman[1]; Jennifer Franks[1]; Jeremy Rouse[1]; Kirsten Romero[2]; Eric Yearley[1]; David Scott[1]; Michael Guerrero[1]; Clayton Beard[1]; *[1]BridgeBio Gene Therapy, Raleigh, NC; [2]BeiGene, Cambridge, MA*

MP 060 **The Urinary Post-translational Modification Landscape and Applications in Clear Cell Renal Cell Carcinoma Biomarker Discovery**; Daniel J Geiszler[1]; Nazlı Ezgi Özkan-Küçük[1]; Gamze Nur Yapici[1]; Murat Can Kiremit[1]; Nurhan Ozlu[1]; *[1]Koc 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 Wang[3]; Anna Malovannaya[3]; Raj Kumar[4]; Dean P Edwards[3]; Patrick R Griffin[1, 2]; *[1]Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; [2]The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL; [3]Baylor College of Medicine, Houston, TX; [4]Touro 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 Yuan[1]; Lisha Xia[1]; Chenxi Wang[1]; Liping Sun[1]; Wenqing Shui[1]; *[1]ShanghaiTech University, Shanghai, China*

MP 064 **Evaluation of viral and allergenic protein complexes by dual cleavable crosslinking technology (DUCCT)**; Akash Talukder[1]; Fnu Ashima[1]; Adway O. Zacharias[1]; Saiful M Chowdhury[1]; *[1]University of Texas at Arlington, Arlington, TX*

MP 065 **Expanding the protein crosslinking tool kits by developing a tyrosine reactive crosslinker**; Adway O. Zacharias[1]; Saiful Chowdhury[2]; *[1]University of Texas at Arlington, Arlington, TX; [2]Univerisity of Texas at Arlington, Arlington, TX*

MP 066 **Characterization of Protein-Protein Interactions by Quantitative Cross-linking Mass Spectrometry in Alzheimer's Disease**; Zexin Zhu[1]; Bin Wang[1]; Xiaofang Zhong[1]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison, School of Pharmacy, Madison, WI; [2]University of Wisconsin-Madison, Department of Chemistry, Madison, WI*

MP 067 **Structural interactomic profiling of the synapse by cross-linking mass spectrometry**; Ke Wang[1]; Cong Wang[1]; Ying Zhu[1]; Fan Liu[1]; *[1]Leibniz-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 Sun[1]; Sergei Khrapunov[1]; Subray Hegde[1]; Simone Sidoli[1]; Michael Brenowitz[1]; *[1]Albert Einstein College of Medicine, Bronx, NY*

MP 069 **FOX Photolysis System-Generated Carbene Footprinting of Peptides**; Lyle W Tobin[1]; Sandeep K. Misra[2]; Joshua S. Sharp[2]; *[1]University of Mississippi, University; [2]University of Mississippi, University, MS*

MP 070 **Structural mass spectrometry justification of AlphaFold generated PsbS structure on the elongated stromal loop region**; Manjula Mummadisetti[1]; Yanchun Lin[2]; Masakasu Iwai[3, 4]; Krishna K Niyogi[3, 4]; Michael L. Gross[2]; Haijun Liu[5]; *[1]Bioagilytix, Raleigh, NC; [2]Department of Chemistry, Washington University in St. Louis, St. Louis, MO; [3]Department of Plant and Microbiology, University of California, Berkeley, Berkeley, CA; [4]Molecular Biophysics and Integrated Bioimaging Divisioin, Lawrence Berkeley National Laboratory, Berkeley, CA; [5]Department 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 Chernev[1]; Timo Sachsenberg[3, 4]; Monika Raabe[1]; Arslan Siraj[3, 4]; Aditi Sharma[5]; Bernard Delanghe[5]; Rosa Viner[6]; Oliver Kohlbacher[3, 4]; Henning Urlaub[1, 2]; *[1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; [2]Institute for Clinical Chemistry, University Medcial Center Göttingen, Göttingen, Germany; [3]Applied Bioinformatics, Department for Computer Science, University of Tübingen, Sand 14, 72076, Tübingen, Germany; [4]Institute of Bioinformatics and Medical Informatics, University of Tübingen, Tübingen, Germany; [5]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [6]ThermoFisher Scientific, San Jose, California*

MP 072 **Exploring an alternative cysteine-reactive chemistry to enable proteome-wide PPI analysis by cross-linking mass spectrometry**; Fenglong Jiao[1]; Leah J. Salituro[2]; Clinton Yu[1]; Craig B. Gutierrez[1]; Scott D. Rychnovsky[2]; Lan Huang[1]; *[1]Department of Physiology and Biophysics, University of California, Irvine, IRVINE, CA; [2]Department 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 Cheng[1]; Emily Chea[1]; Jiana Duan[1]; Sandeep K. Misra[2]; Scot Weinberger[1]; Joshua S. Sharp[1, 2]; *[1]GenNext Technology, Half Moon Bay, CA; [2]University of Mississippi, University, MS*

MP 074 **Mass Spectrometric Footprinting of Protein Adsorption and Desorption at Chromatographic Interfaces**; Kimber N. Focke[1]; Brian T. Cooper[1]; *[1]UNC 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 Chai[1]; Sarah Burris-Hiday[2]; Emily E. Scott[2]; Michael L. Gross[1]; *[1]Washington University in St.Louis, Saint Louis, MO; [2]University of Michigan, Ann Arbor, MI*

MP 076 **AZURIN: A MODEL METALLOPROTEIN TO STUDY AN OLIGOMERIZATION PROCESS**; Roman Tuzhilkin[1]; Vladimir Ondruska[1]; Jiri Hudecek[1]; Miroslav Sulc[1]; *[1]Department of Biochemistry, Charles University, Prague, Czech Republic*

MP 077 **Crosslinking-MS Captures Transient Interactions within Phase Separated Viral Replication Factories**; Nicole D. Wagner[1]; Austin B. Moyle[1, 2]; Chao Wu[3]; Gaya K. Amarasinghe[3]; Daisy W Leung[3]; Michael L Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]AbbVie Inc., North Chicago, IL; [3]Washington University School of Medicine, St. Louis, MO*

MP 078 **Kinase phosphoprobing for profiling protein conformational changes**; Asato Maeda[1]; Kosuke Ogata[1]; Naoyuki Sugiyama[1]; Yasushi Ishihama[1, 2]; *[1]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; [2]National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan*

MP 079 **Characterization of Varroa destructor proteins targeted by new acaricides.**; Osei Boakye Fordwour[1]; Leonard

Foster[1]; Erika Plettner[2]; *[1]UBC, Vancouver; [2]Simon Fraser University, Burnaby, BC*

MP 080 **Towards a global phosphoproteomic map of chemotherapy-specific signaling responses**; William Comstock[1]; Ethan J Sanford[1]; Yiseo Rho[1]; Marcus Bustamante Smolka[1]; *[1]Cornell University, Ithaca, NY*

MP 081 **Comprehensive proteome analysis of few neutrophils exposed to melanoma cells of various aggressiveness**; Susmita Ghosh[1]; Zülal Cibir[2]; Laxmikanth Kollipara[3]; Matthias Gunzer[1, 2]; Albert Sickmann[1]; *[1]Leibniz Institute for Analytical Sciences - ISAS, Dortmund, Germany; [2]University of Duisburg-Essen, Essen, Germany; [3]Leibniz 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 Luu[1]; Chang Ge[2]; Yisha Tang[2]; Andrew K Godwin[3, 4]; Judith Su[5]; Laura M Sanchez[1]; *[1]University of California Santa Cruz, Santa Cruz, CA; [2]University of Arizona, Tuscon, AZ; [3]University of Kansas Medical Center, Kansas City, KS; [4]University of Kansas Cancer Center, Kansas City, KS; [5]University 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 Ogbonna[1]; Hisanao Hazama[1]; Katsuyoshi Masuda[1, 2]; Kunio Awazu[1, 3]; *[1]Graduate School of Engineering, Osaka University, Suita, Japan; [2]Graduate School of Medicine, Kyoto University, Kyoto, Japan; [3]Global 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 Shah[1]; Deng Pan[2]; Joanna Bons[1]; Jacob P. Rose[1]; Rosemary Bai[2]; Chira Chen-Tanyolac[2]; Xianhong Wang[2]; Veena Sangwan[3]; Sophie Camilleri-Broët[4]; Philippe Gascard[2]; Lorenzo Ferri[3]; Thea D Tlsty[2]; Birgit Schilling[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]Department of Pathology, University of California, San Francisco, CA; [3]Division of Thoracic and Upper Gastrointestinal Surgery, Montreal General Hospital, McGill University Health Centre, Montreal, QC; [4]Department 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 Perez[1]; Joohyun Ryu[2]; Mihir Shetty[3, 4]; Boris Winterhoff[3, 4]; Timothy K. Starr[3, 4]; Stefani N. Thomas[2]; *[1]Microbiology, Immunology, and Cancer Biology Program, University of Minnesota, Minneapolis, MN; [2]Department of Laboratory Medicine and Pathology, University of Minnesota, Minneapolis, MN; [3]Department of Obstetrics, Gynecology and Women's Health University of Minnesota, Minneapolis, MN; [4]Masonic 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 Bons[1]; Deng Pan[2]; Samah Shah[1]; Rosemary Bai[2]; Chira Chen-Tanyolac[2]; Nathan Basisty[1]; Amy O'Broin[1]; Jacob P. Rose[1]; Veena Sangwan[3]; Sophie Camilleri-Broët[4]; Philippe Gascard[2]; Lorenzo Ferri[3]; Thea D. Tlsty[2]; Birgit Schilling[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]Department of Pathology, University of California, San Francisco, CA; [3]Division of Thoracic and Upper Gastrointestinal Surgery, Montreal General Hospital, McGill University Health Centre, Montreal, QC; [4]Department of Pathology, McGill University, Montreal, QC*

MP 087 **Intra- and Inter-Patient Tumor Proteome Heterogeneity in Metastatic Lung Cancer**; Sudhir Putty Reddy[1]; Hilal Ozakinci[1]; Lamees Saeed[1]; Bin Fang[1]; Victoria Izumi[1]; Joseph Johnson[1]; Brooke Smedley[1]; Eric Welsh[1]; Steven Eschrich[1]; Eric Haura[1]; Theresa Boyle[1]; John M Koomen[1]; *[1]H. Lee Moffitt Cancer Center, Tampa, FL*

MP 088 **Surfaceome Enrichment Strategies for Discovery of Immunotherapy Targets in Multiple Myeloma**; Bin Fang[1]; Eric Welsh[1]; Umasangtongkul Sura-Attha[1]; Mark Meads[1]; Meghan Menges[1]; Alugubelli Raghunandan Reddy[1]; Frederick Locke[1]; Ken Shain[1]; John M Koomen[1]; Ciara L Freeman[1]; *[1]H. Lee Moffitt Cancer Center, Tampa, FL*

MP 089 **Spatially resolved multi-omic imaging of glioblastoma multiforme to examine hypoxic signatures**; Caroline Pollard[1]; Rory T Steven[2]; Alina Finch[3]; Laura Porto[3]; Victoria Wykes[3]; Colin Watts[3]; Sabrina Nayer[4]; Joe Flint[4]; Jack McMurray[4]; Andrew Filer[4]; Daniel A Tennant[5]; Josephine Bunch[2]; *[1]National Physical Laboratory, Teddington, United Kingdom; [2]National Physical Laboratory, Teddington, United Kingdom; [3]Institute of Cancer and Genomic Science, University of Birmingham, Birmingham, United Kingdom; [4]Institute of Inflammation and Ageing, University of Birmingham, Birmingham, United Kingdom; [5]Institute 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 Cho[1]; Miseon Jeong[1]; *[1]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 Kucsma[3]; Richard Schäffer[1]; Zsuzsanna Szegő[1]; Attila Egri[1]; Gitta Schlosser[2]; Gergely Szakács[3, 4]; Bálint András Deák[5]; Júlia Balog[1]; *[1]Waters Research Center, Budapest, Hungary; [2]ELTE Eötvös Loránd University, Budapest, Hungary; [3]ELKH Research Centre for Natural Sciences, Institute of Enzymology, Budapest, Hungary; [4]Center for Cancer Research, Medical University of Vienna, Vienna, Austria; [5]Department 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-Stavrakaki[1]; Annalisa Lorenzato[2]; Daniel Simon[1]; Yuchen Xiang[1]; Mariangela Russo[2]; Andrew Campbell[3]; Owen Sansom[3]; Alberto Bardelli[2]; Zoltan Takats[1]; *[1]Imperial College London, London, United Kingdom; [2]University of Turin, Turin, Italy; [3]Beatson Institute for Cancer Research, Glasgow, United Kingdom*

MP 093 **Proteomic Signatures for Diagnosing and Monitoring Treatment of Human Bladder Cancer**; Onika Noel[1]; Susan T. Weintraub[1]; Harshit Garg[1]; Furkan Dursun[1]; Dharam Kaushik[1]; Sammy Pardo[1]; Dana Molleur[1]; Michael Liss[1]; Robert Svatek[1]; Ahmed Masour[1]; *[1]Univ. 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. Hovey[1]; Mallory I Frederick[2]; Jenica H Kakadia[2]; Tingting Wu[1]; Courtney Voss[1]; Ilka U Heinemann[1]; Shawn S.C. Li[1]; *[1]Univeristy of Western Ontario, London, ON; [2]University of Western Ontario, London, ON*

MP 095 **Prolyl Isomerase Pin1 is involved in regulating PML-NB dynamics during senescence**; Rodrigo Mohallem[1]; Uma K Aryal[1]; *[1]Purdue 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. Litzi[2, 3, 4]; Neil T. Phippen[2]; Emanuel F. Petricoin[6]; Uma N.M. Rao[2, 3]; G. Larry Maxwell[1, [2, 4]; Thomas P. Conrads[1, 2, 4]; *[1]Women's Health Integrated Research Center, Inova Women's Service Line, Inova Health System, Annandale, Virginia; [2]Women'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; [3]The Henry M. Jackson Foundation for the Advancement of Military Medicine, Inc., Bethesda, Maryland; [4]The John P. Murtha Cancer Center Research Program, Department of Surgery, Uniformed Services University, Bethesda, Maryland; [5]Women'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; [6]Center 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-1/2wildtype high-grade serous ovarian cancer**; Jolene M Duda[1]; Stefani N. Thomas[1]; *[1]University 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'Neill[1]; Evangelos Liapis[1]; Annapurna Pamreddy[1]; Allison Maas[1]; Derek Hanson[1]; Claire Louise Carter[1]; *[1]Hackensack 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 Ahn[5]; Julius Benicky[6, 7]; Thomas P. Conrads[1, 2, 4]; Radoslav Goldman[6, 7, 8]; *[1]Women'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; [2]Women's Health Integrated Research Center, Inova Women's Service Line, Inova Health System, Annandale, Virginia; [3]The Henry M. Jackson Foundation for the Advancement of Military Medicine, Inc., Bethesda, Maryland; [4]The John P. Murtha Cancer Center Research Program, Department of Surgery, Uniformed Services University, Bethesda, Maryland; [5]Department of Biostatistics, Bioinformatics and Biomathematics, Georgetown University, Washington, DC; [6]Department of Oncology, Lombardi Comprehensive Cancer Center, Georgetown University, Washington, DC; [7]Clinical and Translational Glycoscience Research Center, Georgetown University, Washington, DC; [8]Department of Biochemistry and Molecular & Cell Biology, Washington, DC*

MP 100 **Metabolomic profiling of patient-matched primary and recurrent glioblastoma reveals dynamic metabolic reprograming through therapy**; Olivia Taverniti[1]; William D. Gwynne[1]; Andrew T. Quaile[1]; William T. Maich[2]; Zsolt Zador[2]; Sheila K. Singh[2]; J. Rafael Montenegro-Burke[1]; *[1]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; [2]Center 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 Son[1]; Antonia Zamacona Calderon[1]; Adetunji Toriola[2]; Young Ah Goo[1]; *[1]MTAC, MGI, Washington University School of Medicine in Saint Louis, Saint Louis, MO; [2]Washington 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 Liebenberg[1]; Erin Craig[2]; Meredith L Spradlin[1]; Michael F Keating[1]; Robert Tibshirani[2]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Houston, TX; [2]Stanford University, Stanford, CA*

MP 103 **Therapeutic targeting of lipid saturation in recurrent MYC-amplified medulloblastoma.**; William D. Gwynne[1]; Jeremy K Chan[1]; Stefan Custers[2]; Andrew T Quaile[1]; Chitra Venugopal[2]; Sheila K. Singh[2]; J. Rafael Montenegro-Burke[1]; *[1]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; [2]Center 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 Yang[1]; Daniel R. Crooks[1]; Laura S. Schmidt[1, 2]; Richard M. Higashi[3]; Teresa W-M. Fan[3]; Andrew N. Lane[3]; Youfeng Yang[1]; Cathy D. Vocke[1]; W. Marston Linehan[1]; *[1]Urologic Oncology Branch, Center for Cancer Research, National Cancer Institute, National Institutes of Health, Bethesda, Maryland; [2]Basic Science Program, Frederick National Laboratory for Cancer Research, Frederick, Maryland; [3]Department 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 Waas[1]; Christina Karamboulas[2]; Laurie Ailles[2, 3]; Thomas Kislinger[1, 2]; *[1]Princess Margaret Cancer Centre, Toronto, ON; [2]University of Toronto, Toronto, ON; [3]Princess Margaret Cancer Centre, University Health Network, Toronto, ON*

MP 106 **Characterization of Metabolic Heterogeneity in Pediatric Hepatoblastoma**; Trevor M. Godfrey[1]; Andres F. Espinoza[1, 2]; Sarah E. Woodfield[1, 2]; Sanjeev A. Vasudevan[1, 2]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Houston, TX; [2]Texas Children's Hospital, Houston, TX*

MP 107 **Preoperative Classification of Thyroid Nodules by DESI-MS Imaging of Fine Needle Aspiration Biopsies**; Rachel J. Dehoog[1]; Ahmed Al-Fartosi[1]; Neda Zarrin-Khameh[1]; Rongrong Huang[1]; Livia S. Eberlin[1]; James Suliburk[1]; *[1]Baylor 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 Liu[1]; Xiaofen Yuan[1]; Weijia Wu[1]; Huafen Liu[1]; *[1]Calibra Diagnostics, Hangzhou, China*

MP 109 **Classifying membranous nephropathy by mass spectrometry**; Aaron J Storey[1]; Samar Hassen[2]; Christian Herzog[1]; John M Arthur[1]; Rick D Edmondson[1]; Tiffany N Caza[2]; Chris P Larsen[2]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR; [2]Arkana Laboratories, Little Rock, AR*

MP 110 **Mass Spectrometry Imaging Guided Spatial Proteomics for Stratification of Patient with Glioblastoma and Identification of Prognosis Markers**; Marie Duhamel[1]; Maxence Wisztorski[1]; Isabelle Fournier[1]; Michel Salzet[1]; *[1]PRISM 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-Vargas[1]; James Lapalme[1]; Elizabeth Bair[1]; Ona Adair[1]; Nicolas Epie[1]; *[1]South Carolina Public Health Laboratory, Columbia, SC*

MP 112 **Finger-Sticking Good: Clinical Fatty Acids GC-MS Analysis from a Dried Microsample**; Meghan Bradley[1]; Matthew L. Crawford[1]; Christopher M. Shuford[1]; Russell P. Grant[1]; *[1]LabCorp, Burlington, NC*

MP 113 **Adapting the MasSpec Pen for Non-destructive Screening of Oral Premalignancies (OPMDs) to Identify Oral Cavity Squamous Cell Cancers (OCSCC)**; Charles A. Wolfe[1]; Michael F. Keating[2]; Gabrielle Wolter[3]; Erich M. Sturgis[3]; Carlos Chone[4]; Livia S. Eberlin[1]; *[1]Department of Surgery, Baylor College of Medicine, Houston, TX;*

[2]University of Texas at Austin, Austin, TX; [3]Department of Otolaryngology, Baylor College of Medicine, Houston, Texas; [4]Department of Otolaryngology, University of Campinas, Campinas, Brazil

MP 114 **Multiplexed targeted assay for detection of sphingolipids**; Seul Kee Byeon[1]; Kimiyo Raymond[1]; Devin Oglesbee[1]; Matthew Schultz[1]; Dietrich Matern[1]; Akhilesh Pandey[1]; *[1]Mayo Clinic, Rochester, MN*

MP 115 **Microprobe-Capture In-Emitter Elution Coupled with Mass Spectrometry for Structural Elucidation and Clinical Testing of β2-Transferrin**; Ruben Y Luo[1, 2]; Christopher Pfaffroth[2]; Samuel Yang[1]; Kevin Hoang[2]; Priscilla SW Yeung[1, 2]; James Zehnder[1, 2]; Run-Zhang Shi[1, 2]; *[1]Stanford University, Palo Alto, CA; [2]Stanford Health Care, Palo Alto, CA*

MP 116 **Development of 3D Microfluidic Paper-based Analytical devices (μPADs) with Mass Spectrometric Signal Amplification for diagnosis of Malaria in clinical setting**; Ayesha Seth[1]; Abraham Kwame Badu-Tawiah[1]; *[1]The 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 Spectromet**; Dan Liu[1]; Fengmei Hu[2]; Chao Huang[2]; Xianglong Zhao[2]; *[1]Shanghai AB SCIEX, Shanghai, China; [2]China 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 Tan[1]; Troy Puar[1]; Daryl Hee[1]; *[1]Changi 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 Kumar[1]; Lauren Lytwak[1]; Sarah Aijaz[1]; Uma Sreenivasan[1]; *[1]MilliporeSigma, Round Rock, TX*

MP 120 **Rapid Diagnosis of Cytologically Indeterminate Thyroid Fine-Needle Aspiration Biopsies using Paper Spray Ionization Miniature Mass Spectrometry**; Jia-Ying Yu[1]; Laura Min Xuan Chai[1]; Ming-Hsun Wu[2]; Kuen-Yuan Chen[2]; Cheng-Chih Hsu[1]; *[1]National Taiwan University, Taipei, Taiwan; [2]National 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 Zheng[1]; Xinge Cui[1]; *[1]Peking Union Medical College Hospital, Beijing, China*

MP 122 **Quantification of therapeutic proteins with a focus on TDM**; Albert Sickmann[1]; Rob Dahlmann[2, 3]; Phil Carbow[3, 4]; Roman Sakson[4, 5]; Yvonne Reinders[4]; *[1]Leibniz-Institut für Analytische Wissenschaften -, Dortmund, Germany; [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund 44139, Germany, Dortmund, Germany; [3]University of Applied Science, Hamm-Lippstadt,, Hamm, Germany; [4]ISAS- Leibniz Institut für Analytische Wissenschaften, Dortmund, Germany; [5]University of Applied Science, Mannheim, Germany*

MP 123 **Predicting Septic Shock in Emergency Patients with Serum Metabolic Profiles and Machine Learning**; Yu Hong[1]; Li-Hua Li[2]; Ting-Hao Kuo[1]; Yi-Tzu Lee[3, 4]; Cheng-Chih Hsu[1]; *[1]Department of chemistry, National Taiwan University, Taipei, Taiwan; [2]Department of Pathology and Laboratory Medicine, Taipei Veterans General Hospital, Taipei, Taiwan; [3]Department of Emergency Medicine, Taipei Veterans General Hospital, Taipei, Taiwan; [4]Faculty 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 Hu[1]; Dan Liu[2]; Chao Huang[2]; Xianglong Zhao[2]; *[1]Shanghai AB Sciex Analytical Instrument Trading Co.,Ltd.,Shanghai,China, Shanghai, China; [2]Shanghai 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**; Debadeep Bhattacharyya[1]; Patrick McCarthy[1]; Heidi Giese[1]; Martina Werner[1]; Eugenio Daviso[1]; Sameer Vasantgadkar[1]; Ulrich Thomann[1]; *[1]Covaris, Lexington, MA*

MP 126 **Advancing Clinical (Auto)antibody Analysis: Fc-Proteoform Profiling of IgG Allotypes in Rheumatoid Arthritis**; Constantin Blöchl[1]; Christoph Gstöttner[1]; Eva Maria Stork[2]; Rayman T. N. Tjokrodirijo[1]; Peter A. van veelen[1]; Hans Ulrich Scherer[2]; Rene E. M. Toes[2]; Manfred Wuhrer[1]; Elena Domínguez-Vega[1]; *[1]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [2]Department 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 Ferguson[1]; Abraham Kwame Badu-Tawiah[1]; *[1]The 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 Morlacchi[1]; Cate Simmermaker[2]; Patrick Batoon[2]; *[1]Agilent, Lexington, MA; [2]Agilent Technologies, Santa Clara, CA*

MP 130 **Clinical applications utilizing in-pipet dispersive SPE prior to LC-MS/MS**; Yong Chen[1]; Hugh Cramer[2]; M James Ross[1]; Gabriel Odugbesi[2]; *[1]MilliporeSigma, Bellefonte, PA; [2]Millipore Sigma, Bellefonte, PA*

MP 131 **Determination of nine neurotransmitters in plasma by HPLC ESI-MS/MS**; Ruichen Liu[1]; Xuzhe Pei[1]; Chao Huang[1]; Xianglong Zhao[1]; Lihai Guo[1]; *[1]SCIEX, Beijing, China*

MP 132 **High-throughput profiling of reactive cysteines and lysines by automated proteomics workflow**; Zixiang Fang[1]; Taylur P Ma[1]; Hanna G Budayeva[1]; *[1]Genentech, Inc., South San Francisco, CA*

MP 133 **Fast and Sensitive Analysis of FPOP data using MSFragger and FragPipe**; Carolina Rojas Ramirez[1]; Daniel A. Polasky[2]; Jessica Arlett Espino[3]; Lisa Jones[4]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan-Ann Arbor, Ann Arbor, MI; [2]University of Michigan Ann-Arbor, Ann Arbor, MI; [3]University of Maryland, School of Pharmacy, Baltimore, MD; [4]University 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. Wagner[1]; Austin B. Moyle[1, 2]; Nicole D. Wagner[1]; Michael L. Gross[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]AbbVie Inc., North Chicago, IL*

MP 135 **Single Sequence Identification of Probe-Modified Peptides by TrypN C-terminal Clipping of Tryptic Peptides**; Clodette Punzalan[1]; Mariel Clores[1]; Connor Jewell[1]; Xudong Yao[1]; *[1]University of Connecticut, Storrs, CT*

MP 136 **Building fully controlled interactomes and tools to advance protein interaction identification by cross-linking mass spectrometry**; Milan Avila Clasen[1]; Max Ruwolt[2]; Louise Ulrich Kurt[1]; Fabio Cesar Gozzo[3]; Paulo Costa Carvalho[1]; Diogo Borges Lima[2]; Fan Liu[2]; *[1]Laboratory for Structural and Computational Proteomics, Carlos Chagas Institute, Fiocruz, Curitiba, Brazil; [2]Department of Structural Biology, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; [3]Dalton Mass Spectrometry Laboratory, University of Campinas, Campinas, Brazil*

MP 137 **Developing LC-MS workflows for cross-link identification from low sample amounts**; Abigail H Lewis[1]; Siang-Wun Siao[1]; Tomas Koudelka[2]; Julia Kraegenbring[3]; Rosa Viner[4]; Ilaria Piazza[2]; Fan Liu[1]; *[1]Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany; [2]Max Delbrück Center for Molecular Medicine in the Helmholtz Association, Berlin Institute for Medical Systems Biology, Berlin, Germany; [3]Thermo Fisher Scientific, Bremen, Germany; [4]ThermoFisher Scientific, San Jose, CA*

MP 138 **New insight into SARS-CoV-2 interactions with host cells using in vivo Crosslinking Mass Spectrometry**; Martial Rey[1]; Florence GUIVEL-BENHASSINE[2]; Karen Druart[1]; Olivier Schwartz[2]; Julia Chamot-Rooke[1]; *[1]Mass Spectrometry for Biology Unit, Université Paris Cité, Institut Pasteur, CNRS, UAR 2024, Paris, France; [2]Virus and Immunity Unit, Institut Pasteur, Université Paris Cité, CNRS UMR3569, Paris, France*

MP 139 **Comparison of Protein Footprinting Approaches for Epitope Mapping of TNFa/Infliximab complex**; Samantha J Knott[1]; Daniel Benjamin[1]; Richard Y-C Huang[2, 3]; James Dowell[1]; Ekaterina G. Deyanova[2]; Tahmid Hassan[2]; Robert Langish[2]; Yun Wang[2]; Faraz Choudhury[1]; *[1]Immuto Scientific Inc., Madison, WI; [2]Bristol Myers Squibb, Princeton, NJ; [3]Janssen Pharmaceuticals, Spring House, PA*

MP 140 **Probing Antibody-Host Proteome Interactions via Intracellular Cross-linking**; Bradley Hart[1]; Yi He[1]; Lauren M Kraft[2]; Michael Poltash[2]; Chris Sauer[2]; Elsa Gorre[2]; Andrew Mahan[2]; Thomas Kelly[2]; Hirsh Nanda[2]; Rosa Viner[1]; Harsha Gunawardena[2]; *[1]ThermoFisher Scientific, San Jose, CA; [2]JOHNSON 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 Duan[1]; Robert Egan[1]; Calyx Liu[1]; Tyler Fletcher[1]; Emily Chea[1]; Sandeep K. Misra[2]; Joshua Sharp[1, 2]; Scot Weinberger[1]; *[1]GenNext Technology, Half Moon Bay, CA; [2]University of Mississippi, University, MS*

MP 142 **Large scale identification of cross-linked peptides from bovine exosomes using a multi-chromatography approach**; Yiran Ma[1]; Noor H. Naseeb[1]; Adam J Anthony[1]; Andrew D. Couse[1]; Jonathan C. Trinidad[1]; David E. Clemmer[1]; *[1]Indiana University, bloomington, IN*

MP 143 **Benchmarking MS2- and MS3-based acquisition strategies for XL-MS using a developmental ProteinProspector/Touchstone pipeline**; Clinton Yu[1]; Mike Trnka[2]; Peter Baker[2]; Robert Chalkley[2]; Al Burlingame[2]; Lan Huang[1]; *[1]University of California, Irvine, Irvine, CA; [2]University of California San Francisco, San Francisco, CA*

MP 144 **An atlas of reactive and functional chromatin-associated cysteines in cancer**; Daniele Canzani[1]; Brian McEllin[1]; Erin Broderick[1]; Tonibelle Gatbonton-Schwager[1]; Yang Gao[1]; Julia E Robbins[1]; Andrea I Gutierrez[1]; Carolyn Allen[1]; J. Sebastian Paez[1]; William E Fondrie[1]; Lindsay K Pino[1]; Alexander J Federation[1]; *[1]Talus Bioscience, Seattle, WA*

MP 145 **Mapping of the Interaction Site of a Novel Fungal Lectin to a Peptidoglycan from Listera innocua**; Sandeep K. Misra[1]; Sushil K. Mishra[1]; Nika Janez[2]; Robert J. Doerksen[1]; Jerica Sabotič[2]; Joshua S. Sharp[1]; *[1]University of Mississippi, University, MS; [2]Jozef 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 Davisson[1]; Charles Dann[2]; Jonathan C. Trinidad[3]; James Reilly[3]; *[1]Indiana University, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, Indiana; [3]Indiana University Bloomington, Bloomington, IN*

MP 147 **Visualization of transient DOT1A-nucleosome interactions in solution by X-ray protein footprinting**; Janna Kiselar[1]; Victoria S Frisbie[2]; Mark R Chance[1]; Hideharu Hashimoto[2]; Erik W Debler[2]; *[1]Case Western Reserve University, Cleveland, OH; [2]Thomas Jefferson University, Philadelphia, PA*

MP 148 **Applying Machine Learning Tools to Analyze Crosslinking and TMT Mass Spectrometry Datasets**; Zhihui Wen[1]; Ying Zhang[1]; Yan Hao[1]; Laurence Florens[1]; *[1]Stowers 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 Mirzakhanyan[1]; Andris Jankevics[2]; Richard A. Scheltema[2]; Paul D. Gershon[1]; *[1]UC-Irvine, Irvine, CA; [2]Utrecht University, Utrecht, Netherlands*

MP 150 **Enrichable covalent labeling for efficient global, temporal, in situ profiling of protein structural changes in living cells**; Chengzhi Cai[1]; Guoting Qin[1]; Shara Duong[1]; John Mansour[1]; Conor Mullens[2]; *[1]University of Houston, Houston, TX; [2]Bruker 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 Chiang[1]; Ming-Chi Lu[1, 2]; Ning-Sheng Lai[1]; Chien-hsueh Tung[1]; Kuang-Yung Huang[1]; Bao-Bao Hsu[1]; Chih-Chia Yu[2]; Yi-Ling Ye[3]; *[1]Division of Immunology, Allergy and Rheumatology, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan; [2]Department of Medical Research, Dalin Tzu Chi Hospital, Buddhist Tzu Chi Medical Foundation, Dalin, Taiwan; [3]Department of Biotechnology, National Formosa University, Huwei, Taiwan*

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 Florianova[3]; Josiane Lafleur[4]; Adriana Aguilar-Mahecha[4]; Mark Basik[5]; Gerald Batist[1, 4, 6, 7]; Christoph H Borchers[1, 2, 4, 8]; *[1]Division of Experimental Medicine, McGill University, Montreal, QC; [2]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [3]Department of Pathology, Segal Cancer Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [4]Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [5]Department of Oncology and Surgery, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [6]Department of Oncology, McGill University, Montreal, QC; [7]Exactis Innovation, Montreal, QC; [8]Department 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 Karemaker[1]; Roland Bruderer[1]; Jakob Vowinckel[1]; Karel Novy[1]; Kristina Beeler[1]; Raphael Heilig[1]; Sebastian Müller[1]; Lukas Reiter[1]; Yuehan Feng[1]; *[1]Biognosys 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 Burgt[1]; Derk C.F. Klatte[1]; Iris J.M. Levink[2]; Bert A. Bonsing[1]; Wilma E. Mesker[1]; Djuna L. Cahen[3]; Gwenny M. Fuhler[3]; Marco J. Bruno[3]; Monique E. Van Leerdam[1]; Manfred Wuhrer[1]; *[1]Leiden University Medical Center, Leiden, Netherlands; [2]Erasmus Medical Center Rotterdam, Rotterdam, Netherlands; [3]Erasmus Medical Center Rotterdam, Rotterdam, Netherlands*

MP 155 **3-Dimensional Primary Human Chondrocyte Pellets and Cellular Alterations during Osteoarthritis and Senescence**; Jacob P. Rose[1]; Sandip Patel[1]; Joanna Bons[1]; Charles A. Schurman[1]; Christina D. King[1]; Samah

Shah[1]; Judith Campisi[1, 2]; Tamara Alliston[3, 4]; Birgit Schilling[1]; *[1]Buck Institute for Research on Aging, Novato, CA; [2]Lawrence Berkeley Laboratory, University of California, Berkeley, CA; [3]University of California San Francisco, Department of Orthopaedic Surgery, San Francisco, CA; [4]UC Berkeley/UCSF Graduate Program in Bioengineering, Berkeley, CA*

MP 156 **Explore protein glycosylation as non-invasive biomarker for chronic liver diseases**; Mark M. Kushnir[1]; Carmen Dunbar[1]; Yanhong Wu[2]; Yifei Yang[2]; *[1]ARUP Laboratories, Salt Lake City, UT; [2]Mayo Clinic, Rochester, MN*

MP 157 **Combined serum proteome profile of Alzheimer's disease**; Jiayi Zhang[1]; Huali Shen[1]; *[1]Fudan 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. Verhaert[1]; Raf Sciot[2]; Gilles Frache[3]; *[1]ProteoFormiX, Beerse, Belgium; [2]Academic Hospital University of Leuven, Leuven, Belgium; [3]Luxembourg Institute of Science and Technology, Belvaux, Luxembourg*

MP 159 **Investigation of Bile Acids of in Public Data related to Neurological Disorders**; Jasmine Jungok Zemlin[1]; Pieter C Dorrestein[1]; Ipsita Mohanty[1]; *[1]UCSD, La Jolla, CA*

MP 160 **Deep, Unbiased and Quantitative mass spectrometry-based plasma proteome analyses of adaptive response to COVID-19 vaccine**; Ting Huang[1]; Alex Rosa Campos[2]; Ramon Diaz Pena[2]; Svetlana Maurya[2]; Khatereh Motamedchaboki[1]; Laura R. S. Oliveira[3]; Camila I. Alves[3]; Rafael L. Rosa[3]; Yohana P. C. Alves[3]; Lucélia Santi[3]; Walter O. Beys-da-Silva[3]; *[1]Seer, Inc., Redwood City, CA; [2]Sanford Burnham Prebys, San Diego, California; [3]Federal 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 Zhang[4]; Shaomin Zou[4]; Jianhong Chen[5]; Weining Zhao[6]; Guixue Hou[1, 2]; Zeyan Zhong[5]; Jialong Li[4]; Yuhua Ye[4, 7]; Xiangmin Xu[4, 7]; Liang Lin[1, 2]; *[1]BGI Genomics, BGI-Shenzhen, Shenzhen, China; [2]Clinical laboratory of BGI Health, BGI-Shenzhen, Shenzhen, China; [3]BGI Genomics, BGIShenzhen, Shenzhen, China; [4]Department of Medical Genetics, School of Basic Medical Sciences, Southern Medical University, Guangzhou, China; [5]Department of Medical Genetics and Prenatal Diagnosis, Huizhou First Maternal and Child Health Care Hospital, Huizhou, China; [6]College of Pharmacy, Shenzhen Technology University, Shenzhen, China; [7]Innovative 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 Matthews[1]; Aishath Shaufa Shareef[1]; Lee A Gethings[2]; Lisa Reid[2]; Adam King[2]; Stephen Fowler[1]; Angela Simpson[1]; Timothy Felton[1]; Clare Mills[3]; *[1]University of Manchester, Manchester, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom; [3]University 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 Auger[1]; Jean Lacourcière[1]; Jonathan Rochon[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC*

MP 164 **Investigating the discriminatory potential of urinary DNA/RNA adductomics in head-neck cancers patients**; Sachin B Jorvekar[1]; Aishwarya Jala[1]; Sourabh Chouhan[1]; Avdesh Rai[2]; Anupam Das[3]; Kaberi Kakati[3]; Kishore Das[3]; Anupam Sarma[4]; Roshan M Borkar[1]; *[1]National Institute of Pharmaceutical Education and Research-Guwahati, Guwahati, India; [2]DBT Centre for Molecular Biology and Cancer Research, Dr. Bhubaneswar Borooah Cancer Institute,, Guwahati, India; [3]Department of Head and Neck Oncology, Dr. Bhubaneswar Borooah Cancer Institute, Guwahati, Guwahati, India; [4]Department of Onco-Pathology, Dr. Bhubaneswar Borooah Cancer Institute, Guwahati, India*

MP 165 **Metabolite profiling applied to biomarker discovery in pancreatic cancer using high resolution LC-MS/MS**; Alan Barnes[1]; Emily G Armitage[1]; Neil Loftus[1]; Elon Correa[2]; Lynne Howells[3]; Sén Takeda[4]; Wen Chung[5]; *[1]Shimadzu Corporation, Manchester, United Kingdom; [2]Liverpool John Moores University, Liverpool, United Kingdom; [3]Institute for Precision Health, The University of Leicester, Leicester, United Kingdom; [4]Department of Anatomy, Teikyo University School of Medicine, Tokyo, Japan; [5]Leicester 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 Chen[1]; Xuemei Zeng[2]; Carl Bertram[1]; Thomas K Karikari[1]; Nathan A Yates[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]University 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 Gordon[1]; Matt Willetts[2]; Diego Assis[3]; Liwen Zhang[4]; Yanqiao Zhang[5]; *[1]Bruker, Billerica,, MA; [2]Bruker Scientific, LLC, Billerica, MA; [3]Bruker Scientific, Billerica, MA; [4]Ohio State University, Columbus, OH; [5]Northeast Ohio Medical University, Rootstown, OH 44272*

MP 168 **Temporal proteomic analysis of the high containment pathogen Ebola on primary human cells**; William Russell[1]; Ruben Sota Acosta[2]; Lee K Palmer[2]; *[1]University of Texas Medical Branch, Galveston, TX; [2]UTMB at Galveston, Galveston, TX*

MP 169 **In Vivo Digestion Products of Dietary Gluten Proteins as Markers to Study Celiac Disease**; Jennifer A Sealey Voyksner[1]; Robert Voyksner[2]; Jack Syage[3]; Chaitan Khosla[4]; Joseph Murray[5]; *[1]ImmunogenX, Durham, NC; [2]LCMS Limited, Durham, NC; [3]ImmunogenX, Newport Beach, CA; [4]Stanford University, Palo Alto, CA; [5]Mayo Clinic, Rochester, MN*

MP 170 **Comparative analysis of extracellular vesicle low-molecular-weight proteins and peptides of cancer lines**; Aisha Sithika[1]; Vivek Shekar[1]; Adaikkalam Vellaichamy[1]; *[1]Anna 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 Lacourcière[1]; Serge Auger[1]; Jonathan Rochon[1]; Pierre Picard[1]; *[1]Phytronix 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]; *[1]Boston Children's Hospital, Boston, MA; [2]Harvard Medical School, Boston, MA*

MP 173 **Molecular characterization of inverse agonists targeting PPARg in bladder cancer using structural and quantitative proteomics**; Kuang-Ting Kuo[1, 2]; Ruben D. Garcia-Ordonez[3]; Bilel Bdiri[3]; Theodore Kamenecka[3]; Patrick R. Griffin[1, 2, 3]; *[1]The Scripps Research, Jupiter, FL; [2]Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; [3]The 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 Yin[1]; Ronghu Wu[1]; *[1]Georgia 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 Khajavinia[1]; Deborah Michel[1]; Randy W. Purves[1, 2]; Robert Laprarie[1]; Anas El-Aneed[1]; *[1]University* *of Saskatchewan, Saskatoon, SK; [2]Canadian 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 Xue[1]; Alexandra Frommlet[1]; Robert Blake[1]; Alexis Rohou[1]; Melinda Mulvihill[1]; Ke Sherry Li[1]; *[1]Genentech, South San Francisco, CA*

MP 177 **Covalent inhibitor screening of cellular protein targets using mass spectrometry for hit identification in living cells**; Sherry Ke Li[1]; Ryan Conrad[1]; Ryan Raisner[1]; Brett Babin[1]; Jing Xue[1]; Melinda Mulvihill[1]; *[1]Genentech, South San Francisco, CA*

MP 178 **The Limited-Proteolysis method in Drug Development: Powerful workflow to identify drug targets and evaluate drug specificity**; Fabio Sabino[1]; Jaruschka Pecnik[1]; Roland Bruderer[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

MP 179 **Development and validation of an LC-MS/MS method for quantifying occidiofungin in rabbit plasma**; Andrew Cothrell[1]; Ravi Orugunty[2]; James Leif Smith[1, 2]; *[1]Texas A&M University, College Station, TX; [2]Sano Chemicals, College Station, Texas*

MP 180 **Multiplexed CETSA MS as a tool for lead optimization**; Tuomas A Tolvanen[1, 2]; Jennifer A Amrhein[3]; Thomas Hanke[3]; Tomas Friman[1]; Alexey Chernobrovkin[1]; Stefan Knapp[3]; Michael Sundström[2]; Daniel Martinez Molina[1]; *[1]Pelago Bioscience AB, Solna, Sweden; [2]Division of Rheumatology, Department of Medicine Solna, Karolinska University Hospital and Karolinska Institutet, Solna, Sweden; [3]Institute 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 Tang[1]; Qiang Li[2]; Taohong Huang[2]; *[1]Shimadzu?China?Co., Ltd., Chengdu, China; [2]Shimadzu (China) Co., Ltd, Shanghai, China*

MP 182 **Measuring protein thermal stability and phosphorylation changes to capture early cellular responses to small molecule drugs**; Alexey Chernobrovkin[1]; Daniel Martinez Molina[1]; *[1]Pelago Bioscience AB, Solna, Sweden*

MP 183 **Point-of-care quantitation of immunosuppressive drugs in blood by fast microextraction and miniature mass spectrometry analysis**; Yikun Liu[1]; Jinling Lu[1]; Wenpeng Zhang[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China*

MP 184 **The Target Engagement Atlas - Mapping cell biology through small molecule perturbations**; Alexey Chernobrovkin[1]; Tomas Friman[1]; Erin Gilson[1]; Bolette Bossen[1]; Tuomas A Tolvanen[1]; Daniel Martinez Molina[1]; *[1]Pelago Bioscience AB, Solna, Sweden*

MP 185 **Identification of Functionally Relevant and Druggable Protein Targets of Colorectal Cancer Chemoresistance using Protein Folding Stability Profiling**; Baiyi Quan[1]; Morgan A. Bailey[1]; John Mantyh[2]; Hsu S. Hsu[2]; Michael C. Fitzgerald[1]; *[1]Duke University, Durham, NC; [2]Duke 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 Davie[1]; Renmeng Liu[1]; Yiding Hu[1]; Ting Wang[1]; Yurong Lai[1]; *[1]Gilead Sciences, Foster City, CA*

MP 187 **Mass Spectrometry Analysis with Cellular Thermal Shift Assay to Assess Senolytic Pathways in Senescent Monocytes**; Delaney Rutherford[1]; Reema Banarjee[1]; Quinn Strassheim[1]; Amit K Dey[1]; Dimitrios Tsitsipatis[1]; Anjana Ram[1]; Ruin Moaddel[1]; Myriam Gorospe[1]; Nathan Basisty[1]; *[1]National 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 Lamarr[1]; Somayeh Talebzadeh[1]; Jim Breunig[2]; Lars Hanson[2]; Brian Healey[2, 3]; *[1]PureHoney Technologies, Inc., Billerica, MA; [2]Beantown Biotech LLC, Billerica, MA; [3]Revolution Biosciences LLC, Norwell, MA*

MP 189 **Characterization of Hyaluronic Acid-Based Hydrogel Drug Delivery Systems via Online Multimodal Liquid Chromatography-Mass Spectrometry**; Brady W Drennan[1]; Kevin A. Schug[1]; Sam H. Yang[2]; *[1]University of Texas at Arlington, Arlington, TX; [2]Genentech 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 Shi[1]; Sheng-Ping Wang[1]; Lifeng Wang[1]; Fritz Kramer[1]; Wenying Jian[1]; *[1]Janssen 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 Talebzadeh[1]; Zane Thistleford[1]; Can Jon Ozbal[1]; *[1]PureHoney Technologies, Billerica, MA*

MP 192 **The Neuropeptide Neuroparsin-A Regulates Caretaking Behavior in Leafcutter Ants**; Michael Gilbert[1]; Karl Glastad[1]; Maxx Fioriti Fioriti[1]; Tierney Gannon[1]; Matan Sorek[1]; Lindsay Pino[2]; Shelley Berger[1]; Benjamin A Garcia[3]; *[1]University of Pennsylvania, Philadelphia, PA; [2]Talus Bioscience, Seattle, WA; [3]Washington University School of Medicine, St. Louis, MO*

MP 193 **Elucidating the mechanism of germline histone H3.3 mutations on neurodevelopment**; Elizabeth G. Porter[1]; Francisca N. De Luna Vitorino[1]; Khadija D. Wilson[2]; Yixuan (axe) Xie[3]; Peter Klein[2]; Elizabeth J. Bhoj[2]; Benjamin A. Garcia[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]University of Pennsylvania, Philadelphia, PA; [3]Washington 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. Mattamana[4]; Justin E. Bodner[1, 2]; Renu Goel[4]; Daniel R. Foltz[1, 2]; Neil L. Kelleher[1, 2, 3, 4, 5]; *[1]Department of Biochemistry and Molecular Genetics, Northwestern University Feinberg School of Medicine, Chicago, IL; [2]Simpson Querrey Institute for Epigenetics, Northwestern University, Chicago, IL; [3]Chemistry of Life Processes Institute, Northwestern University, Evanston, IL; [4]The Proteomics Center of Excellence, Northwestern University, Chicago, IL; [5]Department 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 Yang[1]; Xiaomei He[1]; Jun Yuan[1]; Chengjie Ma[1]; Yinsheng Wang[1]; *[1]University 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 Ives[1]; Antonin Papin[2]; Alexey A. Soshnev[3]; Kevin Jooss[1]; Navid Ayon[1]; Matt Robey[4]; Ethel Cesarman[2]; Ari M. Melnick[5]; Rafael Melani[1]; Neil L. Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Department of Pathology and Laboratory Medicine, Weill Cornell Medical College, New York, New York; [3]Department of Neuroscience, Developmental and Regenerative Biology, University of Texas at San Antonio, San Antonio, Texas; [4]Proteinaceous, Evanston, Illinois; [5]Department 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 Villalobos[1]; Nicolas L. Young[1]; *[1]Verna & Marrs McLean Department of Biochemistry & Molecular Biology, Baylor College of Medicine, Houston, TX*

MP 198 **Histone proteoform quantitation uncovers the epigenetic response of brown adipose tissue to cold stress**; Bethany C Taylor[1]; Alli M Nuotio-Antar[1]; Nicolas L Young[1]; *[1]Baylor College of Medicine, Houston, Texas*

MP 199 **Scoring Post-translational Modification Crosstalk from Histone Proteoform Data**; Karl Fali Poncha[1]; 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*

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. Fuller[1]; Javier A. Rodriguez-Casariego[2, 3, 4]; Lilian Valadares Tose[1]; Jose M. Eirin-Lopez[2]; Lynne A. Fieber[3]; Francisco A. Fernandez-Lima[1]; *[1]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [2]Department of Biology, Florida International University, Miami, FL; [3]Department of Marine Biology and Ecology, Rosenstiel School, University of Miami, Miami, FL; [4]Neurosciences 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. Paparella[1]; Karl Poncha[1]; Pratim Chowdhury[1]; Ruhee Dere[1]; Cheryl Lyn Walker[1]; Nicolas L. Young[1]; *[1]Baylor 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 Payne[1]; Sue D'Antonio[2]; Mike Adams[3]; Limian Zhao[4]; Anthony Macherone[4]; Greg Thompson[4]; *[1]AnalytEval, SMITHVILLE, TX; [2]Agient Technologies, Cedar Creek, Texas; [3]CWC Labs, Smithville, TX; [4]Agilent 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 Chattopadhaya; *FDA, CVM, Laurel, MD*

MP 205 **Quantifying Insoluble Ferulic Acid and P-Coumaric Acid in Zea mays using LC-MS**; Valeria Zerda Pinto[1]; Alayna Stephens[1]; Cheyenne D Copling[1]; Mary-Margaret B Benware[1]; Tyson Lobb[1]; David Buckley[1]; Patrick S Carney[1]; Hannah Labby[1]; Fatima Romo[1]; Carolyn J Butts-Wilmsmeyer[1]; Kevin R Tucker[1]; Olufunke M Ayegbidun[1]; Ifeoluwa P Osikoya[1]; Logan M Stenger[2]; Laura A Chatham[2]; Tiffany M Jamann[2]; Anthony J Studer[2]; Martin O Bohn[2]; Lucas M Roberts[2]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL; [2]University of Illinois Urbana-Champaign, Urbana and Champaign, IL*

MP 206 **Investigation of Arsenic Accumulation in Deep-frying Oil**; Zhen-yan Li[1]; Zhongping Yao[2]; *[1]HK PolyU, Hung Hom, Hong Kong; [2]HK PolyU, Hung Hom, Hong Kong*

MP 207 **Integrating veterinary drugs and pesticides into a targeted LC-MS/MS exposome-scale biomonitoring method**; Md Zakir Hossain[1]; Yunyun Gu[1]; Max Lennart Feuerstein[1, 2]; Benedikt Warth[1, 2]; *[1]University of Vienna, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Währinger Straße 38, 1090, Vienna, Austria; [2]Exposome 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 Chen[1]; Zou-Xiao Huang[2]; Jung-Wei Chang[3]; Po-Chin Huang[4, 5, 6]; *[1]Department of Chemistry, Tunghai University, Taichung City, Taiwan; [2]Institute of Food Safety and Health, College of Public Health, National Taiwan University, Taipei, Taiwan; [3]Institute of Environmental and Occupational Health Sciences, School of Medicine, National Yang Ming Chiao Tung University, Taipei, Taiwan; [4]National Institute of Environmental Health Sciences, National Health Research Institutes, Miaoli, Taiwan; [5]Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; [6]Department of Medical Research, China Medical University Hospital, China Medical University, Taichung City, Taiwan*

MP 209 **Determination of nitrofuran metabolite residues in shrimp by LC-MS/MS**; Dan Luo[1]; Qiang Li[2]; Hongyuan Hao[3]; Taohong Huang[3]; *[1]Shimadzu (China) Co., LTD, Wuhan, China; [2]Shimadzu （China） Co., LTD, Shanghai, China; [3]Shimadzu (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 Wu[1]; Feng Qin[1]; *[1]PerkinElmer 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]; *[1]SHIMADZU Corporation, Kyoto, Japan; [2]Osaka 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]; *[1]SHIMADZU Corporation, Kyoto, Japan; [2]Osaka 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 Maeshima[1]; Ruth Marfil-Vega[2]; Manami Kobayashi[1]; *[1]SHIMADZU Corporation, Kawasaki, Japan; [2]Shimadzu Scientific Instrument, Columbia, Maryland*

MP 214 **Development of high sensitivity and separation detection method for ciguatoxin analogues by LC/MS/MS**; Manami Kobayashi[1]; Kaoru Nakagawa[2]; Ruth Marfil-Vega[3]; Junichi Masuda[1]; Naomasa Oshiro[4]; *[1]Shimadzu Corporation, Kawasaki-city, Japan; [2]Shimadzu Corporation, Kyoto-city, Japan; [3]Shimadzu Scientific Instruments, Columbia, MD; [4]Division 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 Kim[3]; You Jin Jeon[3]; Hyun Joo An[1, 2]; *[1]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; [3]Department 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 Zhang[1]; Ge Meng[2]; Zhicong Wang[2]; Jianguo Ji[2]; Chunxiao Wang[2]; *[1]Agilent Technologies (Shanghai) Co., Ltd., Shanghai, China; [2]Agilent 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 Westland[1]; Limian Zhao[1]; Bruce Quimby[1]; Anastasia Andrianova[1]; Lakshmi Krishnan[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent 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 Purves[1]; Michelle West[1]; Ratnadipsinh Vaghela[1]; Jana Kinar[1]; Yash Patel[1]; Michael W Belford[2]; Bryn O. Shurmer[1]; *[1]Canadian Food Inspection Agency, Saskatoon, SK; [2]Thermo 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**;

Limian Zhao[1]; Matthew Giardina[2]; [1]*Agilent Technologies, Wilmington, DE;* [2]*Agilent Technologies, Wilmington*

MP 220 **Routine Pesticide Screening Solution: Data Independent Acquisition with a New LC/Q-TOF and Dedicated Screening Software**; Cate Simmermaker[1]; Christian Klein[1]; Karen E Yannell[1]; Kai Chen[1]; Wei Wei[1]; [1]*Agilent Technologies, Santa Clara, CA*

MP 221 **Multi-Residue Pesticide Analysisin Cumin seeds using GC-MS/MS**; Durvesh Sawant[1]; Rahul Dwivedi[1]; Dr. Aseem Wagle[1]; Prashant Hase[1]; Sanket Chiplunkar[1]; Hemant Kesarkar[1]; Dr. Jitendra Kelkar[1]; Dr. Pratap Rasam[1]; [1]*Shimadzu 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 Ma[1]; Suying Li[1]; Zhongping Yao[1]; [1]*The 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 Kitamura[1]; Adriana D'Agostinho[2]; Carolina Mariana Nunes[2]; Dereck Vitali Alves[2]; Roberta Oliveira Servilha[2]; [1]*Shimadzu, Barueri, Brazil;* [2]*Eurofins Special Tests, São Bernardo do Campo, Brazil*

MP 224 **Analytical method for multimycotoxin analysis in cereal grains using an Orbitrap Tribrid mass spectrometer**; Srinivas Sura[1]; Micaela Gray[1]; Jules Carlson[1]; Xiben Wang[1]; Maria Antonia Henriquez[1]; [1]*Agriculture 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 Andrianova[1]; Eric Fausett[1]; Bruce Quimby[1]; Limian Zhao[1]; Joel Ferrer[2]; Aaron Boice[2]; [1]*Agilent Technologies, Wilmington, DE;* [2]*Agilent Technologies, Santa Clara, CA*

MP 226 **Determination of Over 500 Pesticides in Spice by EMR–GPD passthrough cleanup and a Novel Triple Quadrupole LC/MS system**; Hui Zhao[1]; Linfeng Wu[2]; Limian Zhao[1]; Patrick Batoon[2]; [1]*Agilent Technologies, Wilmington, DE;* [2]*Agilent Technologies, Santa Clara, CA*

MP 227 **Ionic Liquid-Based Dispersive Liquid-Liquid Microextraction of Anthelmintic Drug Residues incaprine and ovineMeat Followed by LC-ESI-MS/MS Detection**; Rebagamang Tshepho[1]; Simiso Dube[1]; Mathew M Nindi[1]; [1]*UNISA, Florida Park, Roodepoort, South Africa*

MP 228 **Quantitation of N-nitrosamine impurities in dietary supplement by using LC-MS/MS**; Samruddha Chavan[1]; Nitish Ramchandra Suryawanshi[1]; Nitin Shukla[1]; Nilesh Patil[1]; Purushottam Sutar[1]; Dr. Jitendra Kelkar[1]; Dr. Pratap Rasam[1]; [1]*Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

MP 229 **Qualitative and Quantitative Characterization of Whiskey with Accurate Mass LC MS**; Sue D'Antonio[1]; Nikolas Lau[1]; Greg Thompson[2]; [1]*Agilent Technologies, Cedar Creek, TX;* [2]*Agilent Technologies, Wilmington, Delaware*

MP 230 **Determination of Famphur in Honey by Solid Phase Extraction and Gas Chromatography / Mass Spectrometry**; Seung-Woon Myung; *Kyonggi 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 Benny[1]; Jianbo Liu[1]; [1]*Queens College CUNY, Flushing, NY*

MP 232 **Secondary Proton Transfer during Ion/Ion Reactions between Metal-Adducted Peptides and Fluoranthene**; Darren Gass[1]; Madeline G. Bannon[1]; Michael S. Cordes[1]; Sebastian N. Alberti[1]; Elyssia S. Gallagher[1]; [1]*Baylor University, Waco, TX*

MP 233 **Reprogramming of ETD hardware control to enable ion-ion reactions between electrospray ions**; Jeff Brown[1]; Richard Chapman[1]; Emmy Hoyes[1]; Sarah Brandner[2]; Frederik Lermyte[2]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*Technical University of Darmstadt, Darmstadt, Germany*

MP 234 **Sequencing of Phosphopeptide Anions via Sequential Charge Inversion Ion/Ion Reaction and Electron Capture Dissociation**; David V. Donndelinger[1]; Xinheng Diao[1]; Jonathan T. Specker[1]; Tingting Yan[1]; Boone M. Prentice[1]; [1]*University of Florida, Gainesville, FL*

MP 235 **Enhanced electron-anion interaction in electron-cation neutral plasma: Sequencing of oligonucleotides by electron-detachment dissociation**; Takashi Baba[1]; Kaoru Karasawa[2]; Eva Duchoslav[1]; [1]*SCIEX, Concord, ON;* [2]*AB SCIEX, Shinagawa, Japan*

MP 236 **Ion Parking in Native MS: Spectral Decongestion, Signal Concentration, and Mass Determination**; Nicolas J Pizzala[1]; Scott A McLuckey[2]; Jay S Bhanot[2]; [1]*Purdue University, West Lafayette, IN;* [2]*Purdue University, WEST LAFAYETTE, IN*

MP 237 **Interaction of formates with proton-bound water complexes**; Malick Diedhioiu[1]; Paul Mayer[2]; [1]*University, Ottawa, ON;* [2]*University of Ottawa, Ottawa, ON*

MP 238 **Dehydrogenations of Cyclohexane and Pyrrolidine by M(II) and M(0) Quinoline Complexes (M=Ni and Pd)**; Robert S King[1]; Alexander Buzenski[2]; Richard A. J. O'hair[3]; Allan J Canty[4]; Victor Ryzhov[5]; [1]*Northern Illinois University, Dekalb, IL;* [2]*Northern Illinois University, DeKalb, IL;* [3]*University of Melbourne, Melbourne, Australia;* [4]*University of Tasmania, Hobart, Australia;* [5]*Northern Illinois University (NIU), DeKalb, IL*

MP 239 **New Frontiers for Diserinol Isophthalamide as an Anion Complexation Reagent in Electrospray Ionization Mass Spectrometry**; Madeline Schultz[1]; Sarah L. Parker[1]; Maleesha T. Fernando[1]; Miyuru M. Madduma Wellalage[1]; Neil A. Ellis[1]; Nwanne Dominic Banor[1]; Daniel A. Thomas[1]; [1]*University 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 Fu[1]; Scott A McLuckey[1]; [1]*Purdue University Department of Chemistry, West Lafayette, IN*

MP 241 **Gas-Phase Schiff Base Formation via PAMAM Dendrimer Molecular Containers**; Sarah Nsiah[1]; Scott A McLuckey[2]; [1]*Purdue University, West Lafayette, IN;* [2]*Purdue University, WEST LAFAYETTE, IN*

MP 242 **Acidity of Organic Compounds and Small Peptides in Solution and in the Gas-Phase**; Kim Harvey[1]; Mandy Brinkmann[2]; Michael Browne[2]; Erica Meng[2]; Raj Patel[2]; Jianhua Ren[2]; [1]*University of the Pacific, Stockton, CA;* [2]*University of The Pacific, Stockton, CA*

MP 243 **Selective, gas-phase decarbonylation of formic acid catalyzed by polyoxomolybdate anions**; Howard Z. Ma[1]; Allan J. Canty[2]; Richard A. J. O'hair[1]; [1]*University of Melbourne, Parkville, Australia;* [2]*University of Tasmania, Hobart, Australia*

MP 244 **Computational modelling of reaction intermediates in gas-phase charge inversion ion/ion reactions**; Yingchan Guo[1]; Jonathan T. Specker[1]; Ramón Alain Miranda-Quintana[1]; Boone M. Prentice[1]; [1]*Department 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. Specker[1]; Boone M. Prentice[1]; [1]*University of Florida Department of Chemistry, GAINESVILLE, FL*

MP 246 **Studies of Negative Electron Transfer Dissociation Reagents**; Keaton L Mertz[1]; Katie Kothlow[1]; Michael S. Westphall[2]; John E.P. Syka[3]; Joshua J. Coon[2]; [1]*University of Wisconsin-Madison, Department of Chemistry, Madison, WI;* [2]*University of Wisconsin-Madison, Madison, WI;* [3]*Thermo 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 Kaur[1]; Judy Kuan-Yu Liu[2]; Markus Rohdenburg[3]; Jonas Warneke[3]; Hilkka I.

Kenttämaa[1]; *[1]Purdue University, West Lafayette, IN; [2]Eli Lilly & Company, Indianapolis, IN; [3]University of Leipzig, Leipzig, Germany*

MP 248 **Fragmentation Patterns of Peptoids Containing a Basic Residue**; Ashleigh Ramos[1]; Yadwinder Singh Mann[2]; Jianhua Ren[2]; *[1]University of the Pacific, Stockton, CA; [2]University of The Pacific, Stockton, CA*

MP 249 **Structural elucidation of the 20S Proteasome using native ultraviolet photodissociation mass spectrometry**; Jada N. Walker[1]; Amit Kumar Singh Gautam[2]; Andreas Matouschek[2, 3]; Jennifer S. Brodbelt[1]; *[1]Department of Chemistry, The University of Texas at Austin, Austin, TX; [2]Department of Molecular Biosciences, The University of Texas at Austin, Austin, TX; [3]Institute 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 Dai[1]; Chengjie Ji[1]; *[1]NovaBioAssays, Woburn, MA*

MP 251 **Size-Exclusion Chromatography-Native Mass Spectrometry Coupled with In-Source Denaturation Facilitates Characterization of Biologics for Drug Discovery**; Xiao Guo[1]; Dongdong Wang[1]; *[1]Takeda Pharmaceuticals, Cambridge, MA*

MP 252 **Are Native Conformations of Proteins Preserved Throughout Laser Ablation?**; Neda Feizi Gilandeh[1]; Blessing Chisom Egbejiogu[2]; Kyle L. Wilhelm[1]; Kermit K. Murray[2]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX; [2]Louisiana State University, Baton Rouge, LA*

MP 253 **Structural basis for allosteric modulation of the ABC transporter MsbA by copper(II) and lipid**; Jixing Lyu[1]; Chang Liu[2]; Tianqi Zhang[1]; Samantha Schrecke[1]; Elam P. Nicklaus[1]; Charles Packianathan[1]; Georg K. A. Hochberg[3, 4]; David Russell[1]; Minglei Zhao[2]; Arthur Laganowsky[1]; *[1]Texas A&M University, College Station, TX; [2]University of Chicago, Chicago, IL; [3]Max Planck Institute for Terrestrial Microbiology and Department of Chemistry, University of Marburg, Marburg, Germany; [4]Center 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 Wang[1]; Huishan Li[1]; Nicholas Allen[1]; Ian T Ferraro[1]; Anyin Li[1]; *[1]University 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 Evans[1]; Robert Schrader[2]; Carter Lantz[2]; David H. Russell[2]; *[1]Texas A&M, College Station, TX; [2]Texas A&M University, College Station, TX*

MP 256 **Quantitative Analysis of noncovalent Interactions via LILBID-MS**; Jonathan Schulte[1]; Nina Morgner[1]; Phoebe Young[1]; *[1]Goethe University Frankfurt, Frankfurt am Main, Germany*

MP 257 **Matrix-Landing Mass Spectrometry for Electron Microscopy Imaging of Native Protein Complexes**; Austin Z. Salome[1]; Kenneth W. Lee[1]; Timothy Grant[1]; Michael S. Westphall[1]; Joshua J. Coon[1]; *[1]University of Wisconsin-Madison, Madison, WI*

MP 258 **CDMSAnalysisof Intact 19S, 20S, 26S, and 30S Proteasomes: Evidence for Higher-Order 20S Assemblies at low pH**; Adam J Anthony[1]; Amit K. S. Gautam[2]; Lohra M. Miller[1]; Anya G. Hardwick[1]; Anu Sharma[3]; Subhadip Ghatak[3]; Andreas Matouschek[2]; Martin F. Jarrold[1]; David E. Clemmer[1]; *[1]Indiana University, bloomington, IN; [2]Department of Molecular Biosciences, Austin, TX; [3]Indiana 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. Bergman[1]; Devin M. Makey[1]; Ryan Schroeder[1]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 260 **Improved Signal Processing for Orbitrap Charge Detection Mass Spectrometry**; Michael Goodwin[1]; Kyle Patrick Bowen[1]; Dmitry Grinfeld[1]; Ping Yip[1]; Michael Senko[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 261 **Fluorinated ethylamines as ESI-friendly neutral pH buffers for native mass spectrometry**; Brad Davis[1]; Algirdas Velyvis[1]; Siavash Vahidi[1]; *[1]University 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. Edwards[1]; Michael S. Cordes[1]; Elyssia S. Gallagher[1]; *[1]Baylor University, Waco, TX*

MP 263 **Native ESI MS for Deep Characterization of Target Engagement and Molecular Mode of Action**; Xidong Feng[1]; Wenyi Hua[2]; Jayasankar Jasti[2]; Timothy Foley[2]; Dafydd Owen[2]; Matthew D Troutman[2]; *[1]Pfizer, Groton, CT; [2]Pfizer Inc., Groton, CT*

MP 264 **Multiplexed interrogation of selective inhibitors of fatty acid-binding proteins by native mass spectrometry**; Michelle Q Phan[1]; Indu R Chandrashekaran[1, 2]; Naureen Akhtar[1, 2]; Evgenia Konstantinidou[1, 2]; Thomas Nebl[3]; Darren J Creek[4]; Martin J Scanlon[1, 2]; Raymond S Norton[1, 2]; *[1]Medicinal Chemistry, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Australia; [2]ARC Centre for Fragment-Based Design, Monash Institute of Pharmaceutical Sciences, Monash University, Parkville, Australia; [3]Biology Group, Biomedical Manufacturing Program, CSIRO, Clayton, Australia; [4]Drug 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 Brandner[1]; Tanja Habeck[1]; Frederik Lermyte[1]; *[1]TU 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 Zhou[1]; Jakub Baudys[2]; Ryan Li[3]; Theodore R. Keppel[1]; Sarah H. Osman[2]; Christopher A. Haynes[1]; John R Barr[1]; Dongxia Wang[1]; *[1]Center for Disease Control and Prevention, Atlanta, GA; [2]Centers for Disease Control and Prevention, Atlanta, GA; [3]Augusta 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 Liu[1]; Tyler C Cropley[1]; Olufemi Araoyinbo[1]; Christian Bleiholder[1]; *[1]Florida State University, Tallahassee, FL*

MP 269 **Expanding glycoproteome analysis with Activated-Ion ETD on an Orbitrap Ascend Tribrid**; Annie Jen[1]; Trenton M. Peters-Clarke[2]; Yuchen He[1]; Keaton L. Mertz[2]; Evgenia Shishkova[1, 3]; Michael S. Westphall[1]; Joshua J. Coon[1, 2, 3, 4]; *[1]Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin - Madison, Madison, WI; [3]National Center for Quantitative Biology of Complex Systems, Madison, WI; [4]Morgridge Institute for Research, Madison, WI*

MP 270 **False positive glycopeptide identification through in-FAIMS glycan fragmentation**; Valentina Rangel Angarita[1]; Keira E. Mahoney[1]; Catherine Kwon[1]; Raibat Sarker[1]; Stacy A. Malaker[1]; *[1]Yale University, New Haven, CT*

MP 271 **High Abundance Protein Depletion Combined with Isobaric Tag Boosting Expands N-glycoproteome Coverage in Serum Samples**; Jingwei Zhang[1]; Yuan Liu[1]; Danqing Wang[1]; Zicong Wang[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

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GlcNAcylation and O-GalNAcylation; Senhan Xu[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

MP 273 **Combining selective enrichment and a boosting approach to globally and site-specifically characterize protein co-translational O-GlcNAcylation**; Senhan Xu[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

MP 274 **Anion exchange chromatography-mass spectrometry to characterize alpha-1-acid glycoprotein proteoforms and monitor changes during pregnancy**; Guusje Van Schaick[1]; Manfred Wuhrer[1]; Elena Dominguez Vega[1]; *[1]Center for Proteomics and Metabolomics, LUMC, Leiden, Netherlands*

MP 275 **Spike Glycoprotein S1 Site-specific O-glycosylation: Systematic and Comparative Analysis from Eleven Variants of SARS CoV-2** ; Sherifdeen B Onigbinde[1]; Cristian D Gutierrez Reyes[1]; Mojibola O Fowowe[1]; Oluwatosin E Daramola[1]; Mojgan Atashi[1]; Andrew I. Bennett[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

MP 276 **Quantification of the glycoproteome and surfaceome dynamics during epithelial-to-mesenchymal transition (EMT)**; Xing Xu[1]; Kejun Yin[1]; Zeyu Wang[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

MP 277 **MRM analysis of glycosyltransferases in fibroblasts of CDG patients**; Andreas Harst[1]; Cedric Stahl[2]; Nicole Luebbehusen[1]; Ute Bach[1]; Roman Sakson[3]; Christian Thiel[2]; Thomas Ruppert[1]; *[1]Zentrum fuer molekulare Biologie Heidelberg, Universitaet Heidelberg, Heidelberg, Germany; [2]Heidelberg University Hospital, Heidelberg, Germany; [3]University of applied Science, Mannheim, Germany*

MP 278 **Global analysis of site-specific glycosylation in serum reveals novel candidate biomarker pattern with atypical N-glycosites for diagnosis of hepatocellular carcinoma**; Siyuan Kong[1]; Weiqian Cao[1]; *[1]Institutes of Biomedical Sciences, Fudan University, Shanghai, China*

MP 279 **LC-MS/MS Quantitation of HILIC-Enriched N-glycopeptides derived from low abundance serum glycoproteins in patients with Narcolepsy Type 1**; Mojgan Atashi[1]; Cristian D Gutierrez Reyes[1]; Vishal Sandilya[1]; Waziha Purba[1]; Parisa Ahmadi[1]; Akeem Adeyemi Sanni[1]; Zihan Monshad[1]; Firas Kobeissy[2]; Giuseppe Plazzi[3]; Raffaele Ferri[4]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock; [2]Morehouse School of Medicine (MSM), Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Atlanta, Georgia; [3]Department of Biomedical, Metabolic and Neural Sciences, University of Modena and Reggio Emilia, Modena, Italy; [4]Sleep Research Centre, Department of Neurology IC, Oasi Research Institute- IRCCS, Troina, Italy*

MP 280 **Identifying glycan site profile differences of CD33 expressed in HEK293 and CHO cells**; Kyle Hoffman; *Bioinformatics Solutions Inc, Waterloo*

MP 281 **Investigation of glycosylation of CD209L/L-SIGN and CD209/DC-SIGN and their features as receptors for SARS-CoV-2 infection**; Chaoshuang Xia[1]; Nader Rahimi[1]; Catherine E. Costello[1]; *[1]Boston University Chobanian and Avedisian School of Medicine, Boston, MA*

MP 282 **Identifying Conserved Glycoproteomic Alterations in Clinical Samples and Animal Models of Ureteropelvic Junction Obstruction**; John Froehlich[1, 2]; George Lambrinos[1]; Shannon Dimartino[1]; Alexander Bigger-Allen[1, 2]; Rosalyn Adam[1, 2]; Richard Lee[1, 2]; *[1]Children's Hospital Boston, Boston, MA; [2]Harvard Medical School, Boston, MA*

MP 283 **Mass Spectrometry Analysis of Intact Glycopeptides in Human Clear Cell Renal Cell Carcinoma Tissue Samples**; Fernando Garcia-Marques[1]; Abel Bermudez[1]; Hongjuan Zhao[2]; Rosalie Nolley[2]; James D Brooks[2]; Sharon J Pitteri[1]; *[1]Department of Radiology, Stanford University School of Medicine, Palo Alto, CA; [2]Department of Urology, Stanford University School of Medicine, Stanford, CA*

MP 284 **COVID Spike protein functions are modulated by disulfide linkage patterns. Considerations for vaccine development**; Andrew D Mahan[1]; Alexander N Barnakov[2]; Hirsh Nanda[2]; *[1]Johnson and Johnson, Spring House, PA; [2]Johnson & Johnson, Spring House, PA*

MP 285 **In-depth Characterization of Heterogeneity in Glycoproteoform by Individual Ion Mass Spectrometry (I2MS) and I2MS2**; Jua Lee[1]; Taojunfeng Su[1]; Pei Su[1]; John P. McGee[1]; Steven M. Patrie[1]; Neil L. Kelleher[1]; *[1]Northwestern University, Evanston, IL*

MP 286 **Mapping Low Abundant Serum Glycoproteome Using Ranachrome-5 Immobilized Magnetic Terpolymer as a Super HILIC Sorbent forHepatocellular Carcinoma Biomarker Discovery**; Muhammad Salman Sajid[1]; Habtom Ressom[1]; *[1]Georgetown University, Washington, DC*

MP 287 **Combining orthogonal glycan analysis techniques for a deeper understanding of a tri-specific protein**; Michael McKinnon; *Novartis Institutes for Biomed.Research, Inc., Cambridge, MA*

MP 288 **Hybrid LBA-LC-MS/MS method for glycan-resolved PK monitoring of a therapeutic fusion protein**; Ines C Santos[1]; Brian Melo[1]; Linna Wang[1]; Yury Chaly[1]; Bonnie Wang[1]; Yongjun Xue[1]; Jim Shen[1]; Sekhar Surapaneni[1]; *[1]Bristol Myers Squibb, Princeton, NJ*

MP 289 **New HPLC column for the fast analysis of carbohydrates and glycans by LC-MS**; Hendrik-jan Brouwer[1]; Jean-Pierre Chervet[1]; Christian Marvelous[1]; Thijs Mulder[1]; Martin Eysberg[2]; *[1]Antec Scientific, Alphen a/d Rijn, Netherlands; [2]Antec Scientific, Bostson, MA 02108*

MP 290 **Unraveling the Released N-Glycan Complexity by Implementing High-Resolution Ion Mobility in the HILIC-MS Workflow**; Jordan Stewart[1]; Brandon Nelson[1]; Shahadat Reza[1]; Heidi Vitrac[1]; *[1]MOBILion Systems, Inc., Chadds Ford, PA*

MP 291 **Rapid CE-MS analysis of released N-glycan: optimized workflow for direct CE compatibility**; Patrice Knightly[1]; Sara Carillo[1]; Adi Kulkarni[2]; Erin Redman[2]; Catherine Rawlins[2]; Kate Yu[2]; Jonathan Bones[1]; *[1]National Institute of Bioprocessing Research and Training, Dublin, Ireland; [2]908 Devices, Boston, MA*

MP 292 **ComprehensiveN-glycan Profiling of USP Monoclonal Antibody Reference Standard using GlycanExplorerTMSoftware**; Arun Apte[1]; Rupanjan Goswami[1]; Karthik Kolli[1]; *[1]PREMIER Biosoft, San Francisco, CA*

MP 293 **Characterization of Bile-Salt Stimulated Lipase and Mucin O-glycopeptides by Different Dissociation Techniques**; Joy O Solomon[1]; Sherifdeen B Onigbinde[1]; Cristian D Gutierrez Reyes[1]; Mojibola O Fowowe[1]; Oluwatosin E Daramola[1]; Andrew I. Bennett[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

MP 294 **Application of acoustic ejection coupled to high-resolution mass spectrometry (AE-HRMS) to Metabolite Identification Studies**; Alandra Quinn[1]; Chang Liu[2]; Gordana Ivosev[2]; Carley Heck[1]; Dennis Hyek[1]; George Hajj[1]; Brendon Kapinos[1]; Usa Reilly[1]; *[1]Pfizer, Groton, CT; [2]SCIEX, Concord, ON*

MP 295 **Increasing sensitivity of high throughput host cell protein analysis on a novel high-resolution accurate mass platform**; Eugen Damoc[1]; Tabiwang N. Arrey[1]; Anna Pashkova[1]; Eduard Denisov[1]; Kai Scheffler[2]; Kristina Srzentić[3]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo Fisher Scientific, Germering, Germany; [3]Thermo Fisher Scientific, Reinach, Germany*

MP 296 **Single-shot LC-MS workflow for comprehensive proteome identification on a novel high-resolution accurate mass platform**; Santosh Renuse[1]; Tabiwang N. Arrey[2]; Anna Pashkova[2]; Maowei Dou[3]; Jeff Op De Beeck[4]; Ryan Bomgarden[3]; Bernard Delanghe[2]; Eugen Damoc[2]; Sally Webb[1]; *[1]ThermoFisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific, Rockford, IL; [4]Thermo Fisher Scientific, Ghent, Belgium*

MP 297 **Targeted Whole-Pathway Proteomic Assays with Sample Multiplexing: Data Visualization-Guided Optimization**; Steven R. Shuken[1]; Devin K. Schweppe[1, 2];

Xinyue Liu[1]; Joao A. Paulo[1]; Steven P. Gygi[1]; Qing Yu[1]; *[1]Department of Cell Biology, Harvard Medical School, Boston, MA; [2]Department of Genome Sciences, University of Washington, Seattle, WA*

MP 298 **Developing a Semi-Automated Sample Preparation Method for the Enrichment of Biotinylated Proteins**; Noah Smeriglio[1]; Ashley Frankenfield[1]; Haorong Li[1]; Jiawei Ni[1]; Ling Hao[1]; *[1]Department 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'amico[1]; Gillian E. Robbins[2]; Iris Po[3]; Zichao Fang[3]; Thomas R. Slaney[3]; Li Tao[3]; Gabi Tremml[3]; Brandon T. Ruotolo[2]; Robert T. Kennedy[2]; *[1]Bristol Myers Squibb, Summit, NJ; [2]University of Michigan, Ann Arbor, MI; [3]Bristol Myers Squibb, New Brunswick, NJ*

MP 300 **RTMS: An R Toolkit for Extracting, Analyzing, and Visualizing High-Throughput MALDI Mass Spectrometry Data**; Mary Ashley Rimmer[1]; Nathaniel R Twarog[1]; John Bowling[1]; Brandon Young[1]; Anang A Shelat[1]; Zoran Rankovic[1]; *[1]St. 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 Huang[1]; Nicolas M. Morato[1]; Veronica Feng[1]; Eric T. Dziekonski[1]; R. Graham Cooks[1]; *[1]Purdue University, WEST LAFAYETTE, IN*

MP 302 **Multiplex analysis of bile acids using isobaric labeling with triple quadrupole mass spectrometry**; Suzumi M Tokuoka[1]; Yoshiya Oda[1]; *[1]The University of Tokyo, Tokyo, Japan*

MP 303 **High-throughput and low-volume analysis of native and intact protein mixtures with LAP-MALDI MS**; Bob Challen[1]; Mike Morris[2]; Rainer Cramer[1]; *[1]University of Reading, Reading, United Kingdom; [2]Waters 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 Auger[4]; *[1]Centre Nutriss, INAF, Université Laval, Québec, Qc; [2]CHU de Québec, Université Laval, Québec, Qc; [3]Big Data Research Center, Québec, Qc; [4]Phytronix 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 Kita[1]; Suzumi M Tokuoka[1]; Giorgis Isaac[2]; Lee A Gethings[3]; Robert S Plumb[2]; Yoshiya Oda[1]; *[1]The University of Tokyo, Tokyo, Japan; [2]Waters Corporation, Milford, MA; [3]Waters Corporation, Wilmslow, United Kingdom*

MP 306 **Simultaneous Multi-Omics by Direct Infusion Mass Spectrometry (SMAD-MS)**; Yuming Jiang[1]; Jesse Meyer[2]; *[1]ceders-sinai medical center, Los Angeles, CA; [2]Cedars-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 Bhattacharyya[3]; Kallol Gupta[1, 2]; *[1]Nanobiology Institute, Yale University, West Haven, Connecticut; [2]Yale School of Medicine, Department of Cell Biology, New Haven, CT; [3]Yale School of Medicine, Department of Pharmacology, New Haven, CT; [4]Cancer Biology Institute, West Haven, CT*

MP 308 **Incorporating Ferrimagnetic Beads to High Throughput Affinity Selection Mass Spectrometry**; Jonathan Shrimp[1]; Nate Hoxie[1]; John Janiszewski[1]; Colin Kelly[1]; Matthew Hall[1]; Sam Michael[1]; Meghav Verma[1]; Anton Simeonov[1]; Michael Ronzetti[1]; Bolormaa Baljinnyam[1]; Thomas R. Covey[2]; Peter Kovarik[2]; Chang Liu[2]; Richard Van Breemen[3]; Jianli Zhao[4]; Emmet Welch[4]; Sasikumar Pillai[5]; Subhasish Purkayastha[5]; *[1]NCATS/NIH, Rockville, MD; [2]SCIEX, concord; [3]Oregon State University, Corvallis, OR; [4]Phenomenex, Torrance, CA; [5]Sciex, Framingham, MA*

MP 309 **All-in-One Design and Analysis of Quantitative Studies for High Throughput Experiments**; Richard Lee[1]; Nikki Dare[1]; Nikolay Malashchenok[1]; Karl Demmans[1]; *[1]ACD/Labs, Toronto, ON*

MP 310 **Fully-integrated, high-throughput, dual-stream microflow LC-MS/MS for in vitro screening bioanalysis**; Jamie R Kirsch[1]; Jillian Racich[1]; Daria Vernikovskaya[1]; Brendon Kapinos[1]; Anthony Carlo[1]; Wayne Lootsma[2]; Steve Ainley[2]; *[1]Pfizer Inc., Groton, CT; [2]Sound 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 Imoto[1]; Toshiya Matsubara[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

MP 312 **Ultra-High-Throughput Compound Quality Control with Acoustic Ejection Mass Spectrometry**; Chang Liu[1]; Alandra Quinn[2]; Gordana Ivosev[1]; Robert Mongillo[2]; Bhagyashree Khunte[2]; Brendon Kapinos[2]; *[1]SCIEX, Concord, ON; [2]Pfizer, 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 Picard[1]; Serge Auger[1]; Jean Lacourcière[1]; Jonathan Rochon[1]; *[1]Phytronix 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 Eller[1]; Mitch Wells[1]; Dalton Snyder[1]; Anna Leech[1]; Ann Donnelly[1]; Miranda Jacobs[1]; Jennifer Poole[1]; *[1]Teledyne FLIR, West Lafayette, IN*

MP 315 **A Real-time Informatics Pipeline Enables Screening of Biologics during High-Throughput Expression**; Xianglin Zhai[1]; Behnam Keshavarz[2]; Sidharth Mohan[2]; Bo Zhai[2]; Elsa Gorre[2]; Jing Li[1]; Andrew Mahan[2]; Iman Farasat[2]; Hirsh Nanda[2]; Marshall Bern[1]; Harsha Gunawardena[2]; *[1]Protein Metric Inc., Cupertino, CA; [2]JOHNSON 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 Resager[1]; Marius M Kostelic[2]; Vicki H Wysocki[2]; Marshall Bern[1]; *[1]Protein Metrics, LLC, Cupertino, CA; [2]Ohio State University, Columbus, OH*

MP 317 **Rapid Identification of Changes of Small Molecules in MALDI-MSI Dataof Tumor Spheroids**; Yijia Wang[1]; David Hua[2]; Heather Desaire[2]; Amanda B Hummon[1]; *[1]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; [2]University 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**; Bishoy W Abdelmalak[1]; Lachlan Stuart[1, 2]; Måns Ekelöf[1]; Sergii Mamedov[1]; Lucas Maciel Vieira[1]; Theodore Alexandrov[1, 3, 4, 5]; *[1]Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany; [2]EMBL, Heidelberg, Germany; [3]Metabolomics Core Facility, Heidelberg, Germany; [4]Molecular Medicine Partnership Unit, Heidelberg, Germany; [5]Bio Studio, BioInnovation Institute, Copenhagen, Denmark*

MP 319 **Ion-to-image (i2i) – a new application for unique and rapid processing of mass spectrometry imaging data**; Johan Lillja[1]; Kyle D. Duncan[1, 2]; Ingela Lanekoff[3]; *[1]Uppsala University, uppsala, Sweden; [2]Vancouver Island University, Nanaimo, BC; [3]Uppsala University, Uppsala, Sweden*

MP 320 **iFAMS Imager: A Streamlined Gábor Deconvolution Workflow for Mass Spectrometry Imaging, Protein Localization, and Heatmap Cross-Comparison**; Lily E Miller[1]; Andrew K Swansiger[1]; Manxi Yang[2]; Julia Laskin[2]; James S Prell[1, 3]; *[1]University of Oregon, Eugene, OR;*

[2]Purdue University, WEST LAFAYETTE, IN; [3]Materials Science Institute, University of Oregon, Eugene, OR

MP 321 **Identifying Colocalized Compounds in Mass Spectrometry Images of Diverse Tissue Samples Using Unsupervised Deep Learning**; Emerson Hernly[1]; Rosemary Ajish[1]; Julia Laskin[1]; *[1]Purdue 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. Moens[1]; Lukasz G Migas[1]; David Anderson[2]; Christine A. Curcio[3]; 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]; *[1]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [2]Department of Biochemistry, Vanderbilt University, Nashville, TN; [3]Department of Ophthalmology and Visual Sciences, University of Alabama at Birmingham, Birmingham, AL; [4]Mass Spectrometry Research Center, Vanderbilt University,, Nashville, TN; [5]Department of Chemistry, Vanderbilt University, Nashville, TN; [6]Department of Medicine, Vanderbilt University, Nashville, TN; [7]Department of Pharmacology, Vanderbilt University, Nashville, TN; [8]Department 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) Diao[1]; Zhongling Liang[1]; Yingchan Guo[1]; Boone M. Prentice[1]; *[1]University 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 Liang[1]; Abhisheak Sharma[2]; Christopher R. McCurdy[2]; Boone M. Prentice[1]; *[1]University of Florida Department of Chemistry, GAINESVILLE, FL; [2]College 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 Dreisbach[1]; Carolin M Morawietz[2]; Theodore Alexandrov[3]; Bernhard Spengler[1, 2]; Kerstin Strupat[4]; *[1]TransMIT GmbH, Giessen, Germany; [2]Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Germany; [3]European Molecular Biology Laboratory, Heidelberg, Germany; [4]Thermo 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 Verheggen[2]; Konstantin O. Nagornov[4]; Yury O. Tsybin[4]; Peter D. Verhaert[2]; *[1]MassTech, Columbia, MD; [2]ProteoFormiX, Beerse, Belgium; [3]Barefeet Analytics Private Limited, Pune, India; [4]Spectroswiss, 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 Dexter[1]; Felicia Wirtz[1]; Rory Thomas Steven[1]; Caroline Pollard[1]; Lily Ellis-Gibbings[1]; Stephanie Ling[2]; Richard J A Goodwin[2]; Simon T Barry[2]; Josephine Bunch[1, 3]; *[1]National Physical Laboratory, Teddington, United Kingdom; [2]AstraZeneca, Cambridge, United Kingdom; [3]Imperial College, London, London, United Kingdom*

MP 328 **Innovative Software Solutions for Measuring Analyte Delocalization in MALDI Imaging**; Cole C Johnson[1]; Dalton R Brown[1]; Caitlin M. Tressler[1]; Nathan Riemann[1]; Jason Fan[1]; Kristine Glunde[1]; *[1]Johns 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 Fischer[1]; Ethan Yang[1]; Dawson Miller[2]; Steven S Gross[2]; Qiuying Chen[3]; *[1]Bruker Scientific, LLC, Billerica, MA; [2]Weill Cornell Medicine, New York, NY; [3]Cornell University Medical College, New York, NY*

MP 330 **Statistical Heterospectroscopy of MALDI Imaging and NMR Spectroscopy Data for Evaluation of Breast Tumor Models**; Dalton Brown[1]; Caitlin M. Tressler[1, 2]; Cole Johnson[1]; Sophia Nakuchima[1]; Ethan Yang[1, 2]; Kristine Glunde[1, 2]; *[1]Johns Hopkins AIMS Core, Baltimore, MD; [2]Johns Hopkins School of Medicine, Baltimore, MD*

MP 331 **Metabolite database searching tool in MSiReader for mass spectrometry imaging annotations**; Cristina Arciniega[1]; Tana Palomino[1]; Alexandria L. Sohn[1]; Mary F. Wang[1]; David C Muddiman[1]; *[1]NCSU, Raleigh, NC*

MP 332 **Clustering of mass spectrometry imaging data without dimensionality reduction**; Stanislav Pekov[1, 2, 3]; Mariya Derkach[2]; Anatoly Sorokin[2, 4]; Mariya Shamraeva[2]; Eugene (evgeny) Nikolaev[1]; Igor Popov[2]; *[1]Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; [2]Moscow Institute of Physics and Technology, Dolgoprudniy, Russian Federation; [3]Siberian State Medical University, Tomsk, Russia; [4]Okinawa 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 Trinkle[1]; Emmanuelle Claude[2]; Emrys Jones[2]; Mark Towers[2]; Richard Chapman[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom*

MP 334 **Automated visualization, exploration and material segmentation of ion-mobility mass spectrometry imaging data**; Scott Trinkle[1]; Ayushe Gangal[1]; Joanne Mather[1]; Bindesh Shrestha[1]; Richard Chapman[1]; *[1]Waters Corporation, Milford, MA*

MP 335 **An automated workflow for combining, aligning, exploring, and visualising 3D MS imaging data**; Richard Chapman[1]; Scott Trinkle[1]; Emrys A Jones[2]; *[1]Waters, Milford, MA; [2]Waters, Wilmslow, United Kingdom*

MP 336 **Developing an Expansion Protocol to Improve Spatial Resolution in Mass Spectrometry Imaging**; Li-Cyun Chen[1]; Cheng-Chih Hsu[1]; Chuping Lee[2]; *[1]Cheng-Chih Richard Hsu Lab, Department of Chemistry, National Taiwan University, Taipei City, Taiwan; [2]National 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 Saito[1]; Erika Nagano[2]; Kazuki Odake[2]; *[1]Osaka Univerisity, Suita, Osaka, Japan; [2]Miruion inc, Ibaraki, Osaka, Japan*

MP 338 **Imaging Technologies for Constructing 3D Multimodal Lipid Atlases of the Eye**; David M. G. Anderson[1]; Jeffrey D. Messinger[2]; Dongfeng Cao[2]; Nathan Heath Patterson[3]; Ankita Kotnala[2, 3]; Lukasz G Migas[4]; Raf Van De Plas[3, 4]; Richard M Caprioli[3]; Christine A. Curcio[2]; Kevin Schey[3]; Jeffrey M Spraggins[3]; *[1]Vanderbilt University, Department of Biochemistry, Nashville, TN; [2]University of Alabama at Birmingham, Birmingham, AL; [3]Vanderbilt University, Nashville, TN; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands*

MP 339 **Enhanced high-resolution spatially resolved lipidomics of multicellular tumor spheroids**; Fereshteh Zandkarimi[1]; Rachel C. Avard[1]; Laura J. Kaufman[1]; *[1]Department 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 Lazarek[1]; Vi Tran[1]; Liang Li[1, 2]; *[1]University of Alberta, Edmonton, AB; [2]The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta*

MP 341 **MS3 imaging enables simultaneous mapping of phospholipid C=C and sn-position isomers**; Xiangyu Guo[1]; Aojie Zhang[2]; Wenbo Cao[1]; Qinhua Chen[3]; Wenpeng

Zhang[1]; Zheng Ouyang[1]; [1]*State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University,, Beijing, China; [2]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [3]Shenzhen 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 Miura[3]; Koichi Fukase[2, 3]; Michisato Toyoda[1, 2]; [1]*Department of Physics, Osaka University, Toyonaka, Japan; [2]FRC, Osaka University, Toyonaka, Japan; [3]Department 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]; [1]*State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, Hong Kong SAR, China, Hong Kong, China; [2]Department of Chemistry, Hong Kong Baptist University, Hong Kong, China*

MP 344 **Distribution analysis of galanthamine, a plant alkaloid, by MS imaging**; Kaoru Nakagawa[1]; Tetsuo Iida[1]; Satoshi Kasamatsu[1]; Shuichi Shimma[1, 2]; Manami Kobayashi[1, 3]; [1]*Shimadzu Corporation, Kyoto-city, Japan; [2]Osaka University, Suita-city, Japan; [3]Shimadzu Corporation, Kawasaki-city, Japan*

MP 345 **Sublimated/annealed aminated cinnamic acid analogs for high sensitivity 5µm MALDI IMS of lipids in human tissues**; Martin Dufresne[1]; Angela Kruse[1]; David M. G. Anderson[1]; Lukasz G Migas[2]; Cody Marshall[1]; Katerina V Djambazova[1]; Nathan Heath Patterson[1]; Raf Van De Plas[2]; Richard M Caprioli[1]; Jeffrey M Spraggins[1]; [1]*Vanderbilt University, Nashville, TN; [2]Delft 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 Krupicka[1]; Florent Grelard[1]; Landry Blanc[1]; Julie Arslanoglu[2]; Nicolas Desbenoit[1]; Caroline Tokarski[1]; [1]*Institute of Chemistry and Biology of Membrane and NanoObjects (CBMN), CNRS UMR 5248, Bordeaux Proteome, University of Bordeaux, Bordeaux,, France; [2]Department 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 Yang[1]; Mei-Ling Cheng[1]; [1]*Chang Gung University, Taoyuan, Taiwan*

MP 348 **Development of a single section MALDI-MSI-LC-MS/MS workflow for proteomics and quantitative lipidomics**; Tim Hendriks[1]; Kasper K Krestensen[1]; Giulia Sorbi[2]; Sara Tortorella[2]; Ron M.A. Heeren[1]; Eva Cuypers[1]; [1]*Maastricht MultiModal Molecular Imaging Institute, Maastricht University, Maastricht, Netherlands; [2]Molecular 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 Dreisbach[3]; Karl Christian Schäfer[3]; Carolin M Morawietz[4]; Kerstin Strupat[5]; [1]*Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Gießen, Germany; [2]TransMIT GmbH, Giessen, Germany; [3]TransMIT GmbH, Giessen, Germany; [4]Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Gießen, Germany; [5]Thermo 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 Shen[1]; Ethan Yang[1]; Hoku West-Foyle[1]; Dalton R Brown[1]; Cole C Johnson[1]; LaToya Roker[1]; Caitlin M. Tressler[1]; Ishan Barman[2]; Scot Kuo[1]; Kristine Glunde[1]; [1]*Johns Hopkins University School of Medicine, Baltimore, MD; [2]Johns 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 Roempp[1]; Bastian Jahreis[1]; Oliver Wittek[1]; [1]*Bioanalytical 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. Eberlin[2]; [1]*The University of Texas at Austin, Austin, TX; [2]Baylor College of Medicine, Houston, TX*

MP 353 **Measuring spatial resolution of different Mass Spectrometry Imaging modalities**; Martin Metodiev[1, 2]; Rory Thomas Steven[3]; Angeliki Christakopoulou[3]; Zoltan Takats[2, 4]; Josephine Bunch[2, 3, 4]; [1]*NPL, Teddington, United Kingdom; [2]Imperial College, London, London, United Kingdom; [3]National Physical Laboratory, Teddington, United Kingdom; [4]Rosalind 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 Hapuarachchige[1]; Young Jin Lee[1]; [1]*Iowa 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 Galindo[1]; Natalie Merola[1]; Kristina Jurcic[1]; Steven R. Laviolette[1]; Ken K.-C. Yeung[1]; [1]*Western University, London, ON*

MP 356 **Novel reactive mass tags for the sensitive detection of steroidal ketones by MALDI MSI**; Rachel S. Pryce[1]; Nassim Maarouf[1]; Ayyoub Selka[1]; Dominique Trudel[1]; Fred Saad[1]; Karina Gasbarrino[2]; Stella S. Daskalopoulou[2]; William D. Lubell[1]; Pierre Chaurand[1]; [1]*University of Montreal, Montreal, QC; [2]McGill University, Montreal, Québec*

MP 357 **Characteristics of a new caged matrix with high vacuum stability for MALDI mass spectrometry imaging**; Qiuqin Zhou[1]; Stefano Rizzo[2]; Janina Oetjen[3]; Annabelle Fülöp[1]; Miriam Rittner[2]; Hartmut Gillandt[2]; Carsten Hopf[1, 4, 5]; [1]*CeMOS - Center for Mass Spectrometry and Optical Spectroscopy, Mannheim, Germany; [2]Sirius Fine Chemicals SiChem GmbH, Bremen, Germany; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Medical Faculty of Heidelberg University, Heidelberg, Germany; [5]Mannheim 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 Drake[1]; Minyong Chen[2]; Grace Grimsley[1]; Christopher H Taron[2]; [1]*Medical University of South Carolina, Charleston, SC; [2]New England Biolabs, Inc., Ipswich, MA*

MP 359 **Multi-Site Assessment of the MALDI HiPLEX-IHC Miralys System**; Kyle A Vanderschoot[1]; Emily R. Sekera[2]; Gargey B. Yagnik[3]; Mark J. Lim[3]; Kenneth J. Rothschild[3]; Katherine A. Stumpo[4]; Amanda B. Hummon[2]; Erin H. Seeley[5]; Elizabeth K. Neumann[6]; [1]*University of California, Davis, Davis, CA; [2]The Ohio State University-Comprehensive Cancer Center, Colombus, OH; [3]AmberGen, Inc., Billerica, MA; [4]Bruker Scientific, LLC, Billerica, MA; [5]University of Texas at Austin, Austin, TX; [6]University 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 Lakkimsetty[1]; Andreas Weber[2]; Kylie Ariel Bemis[1]; Melanie Christine Föll[2]; Olga Vitek[1]; [1]*Northeastern University, Boston, MA; [2]University 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**

Mice; Jiaxin Feng[1]; Milagros Suarez[2, 3]; Dallas Freitas[1]; Tingyuan Yang[1]; Xi Chen[1]; Shuli Tang[1]; Yuhan Yang[4]; Xiaonan Li[2, 3]; Yun Huang[4]; Yuchen Du[2, 3]; Xin Yan[1]; *[1]Department of Chemistry, Texas A&M University, College Station, TX; [2]Ann & Robert H. Lurie Children's Hospital of Chicago, Chicago, IL; [3]Robert H. Lurie Comprehensive Cancer Center, Feinberg School of Medicine, Chicago, IL; [4]Center for Epigenetics & Disease Prevention, Texas A&M Institute of Biosciences and Technology, Houston, TX*

MP 362 **On-Tissue Derivatization for enhanced Carbohydrates and Sterols detection in Bombus Impatiens Bee via MALDI mass spectrometry**; Nilay Saha[1]; Andrew Goodenough[1]; Taylor Hatcher[1]; Michael Dillon[1]; Franco Basile[1]; *[1]University of Wyoming, Laramie, WY*

MP 363 **Optimization of embedding media for MALDI-mass spectrometry imaging of frozen tissue**; Ching-Yuan Yang[1]; Yatao Shi[2]; Yuan Liu[2]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

MP 364 **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 365 **Unified and standardized mass spectrometry data processing in Python using spectrum_utils**; Wout Bittremieux[1]; Lev Levitsky[2]; Mateo Pilz[3]; Timo Sachsenberg[3]; Florian Huber[4]; Mingxun Wang[5]; Pieter C Dorrestein[6]; *[1]University of Antwerp, Antwerpen, Belgium; [2]Moscow institute of physics and technology, Moscow, Russia; [3]University of Tübingen, Tübingen, Germany; [4]Hochschule Düsseldorf, Düsseldorf, Germany; [5]University of California Riverside, Riverside, CA; [6]University of California San Diego, San Diego, CA*

MP 366 **Improved identification of isomers using the High Dimensional Consensus Mass Spectral similarity algorithm**; Deborah F McGlynn[1]; Jason Eveleth[1, 2]; Nirina Rabe Andriamaharavo[1]; Anthony Kearsley[1]; *[1]National Institute for Standards and Technology, Gaithersburg, MD; [2]Brown University, Providence, RI*

MP 367 **Novel DNN-powered quadrupole isolation profile analysis algorithm for improved speed, measurement robustness, and quality control**; Adrian Schütz[1]; Amelia Peterson[1]; Bastian Reitemeier[1]; Bernd Hagedorn[1]; *[1]Thermo Fisher Scientific, Bremen, Germany*

MP 368 **High-throughput plasma proteomics to identify diabetes associated protein biomarkers and pQTLs**; Harendra Guturu[1]; Guhan Venkataraman[1]; Amir Alavi[1]; Ryan Benz[1]; Khatereh Motamedchaboki[1]; Anna Halama[2]; Frank Schmidt[2]; Karsten Suhre[2]; Serafim Batzoglou[1]; *[1]Seer, Inc., Redwood City, CA; [2]Weill Cornell Medicine - Qatar, Education City, Qatar*

MP 369 **Crema: an open-source Python tool for target-decoy false discovery rate estimation**; Andy Lin[1]; Donovan See[2]; Uri Keich[3]; William E Fondrie[4]; William Stafford Stafford[2]; *[1]Pacific Northwest National Laboratory, Seattle, WA; [2]University of Washington, Seattle, WA; [3]University of Sydney, Sydney, Australia; [4]Talus Bioscience, Seattle, WA*

MP 370 **An automated computational pipeline for retention time alignment across LC systems**; Ian Reah[1]; Scott Trinkle[2]; Ryan P Marchand[2]; Chris Preston[1]; Ian Morns[1]; Richard Chapman[2]; Paul Fitch[2]; *[1]Waters Corporation, Newcastle upon Tyne, United Kingdom; [2]Waters Corporation, Milford, MA*

MP 371 **Statistical analysis of tandem mass spectra**; Felix Servant[1, 2]; Alexandre Giuliani[1, 2]; Laurent Nahon[1]; *[1]Synchrotron SOLEIL, L'Orme des Merisiers, Départementale 128, 91190 Saint-Aubin, France, Saint-Aubin, France; [2]INRAE, UAR1008, Transform Department, Rue de la Géraudière, BP 71627,44316 Nantes, France, Nantes, France*

MP 372 **Relative Probabilities of Library Search: A Comprehensive analysis of NIST/EPA/NIH EI and Tandem Libraries**; Adva Baratz[1]; Stephen E Stein[2]; *[1]Israel Institute for Biological Research, Ness-Ziona, Israel; [2]NIST, Gaithersburg, MD*

MP 373 **Enhancing compound identification workflows with a novel library manager software application**; Elizabeth Almasi[1]; Emma E Rennie[1]; James S Pyke[1]; Tristan Chutka[1]; Andrew McEachran[1]; *[1]Agilent Technologies, Santa Clara, CA*

MP 374 **Sin.R: A SAINT-like AP-MS protein-interaction score implemented in R**; Manor Askenazi[1]; Beatrix Ueberheide[2]; Jackeline Ponce[2]; *[1]Biomedical Hosting LLC, Arlington, MA; [2]NYU Langone Health, New York, NY*

MP 375 **MetaproDec: a new algorithm to appraise the quantitative composition of a microbiome based upon metaproteome**; Jiahua Mu[1, 2]; Hongkai Xu[1, 2]; Yuxing Zhang[2]; Yamei Deng[2]; Da Qi[2]; Siqi Liu[1, 2]; *[1]College of Life Sciences, University of Chinese Academy of Sciences, Beijing, China; [2]Center of Proteomic Analysis, BGI Life Science Research Institute, Shenzhen, China*

MP 376 **How well did you trap that ion? Find out with PeptidePrisoner!**; Luis Mendoza[1]; Michael R. Hoopmann[2]; Eric W. Deutsch[2]; Robert L. Moritz[2]; *[1]Institute For Systems Biology, Seattle, WA; [2]Institute for Systems Biology, Seattle, WA*

MP 377 **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 378 **Optimal transport-based LC-MS alignment algorithm**; Stanisław Jan Grodzki[1]; Justyna Paulina Król[1]; Michał Piotr Startek[1, 2]; Anna Barbara Gambin[1]; *[1]Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; [2]Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany*

MP 379 **Triqler for Data Independent Aquisition Data**; Patrick Truong[1]; Matthew The[2]; Lukas Kall[1]; *[1]Royal Institute of Technology, Stockholm, Sweden; [2]Technical University of Munich, Freising, Germany*

MP 380 **Estimating relative concentrations of analytes using computational optimal transport**; Michal A. Ciach[1, 2]; Barbara Domżał[1]; Michał Piotr Startek[1, 3]; Grzegorz Skoraczyński[1]; Dirk Valkenborg[2]; Błażej Miasojedow[1]; Anna Barbara Gambin[1]; *[1]Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; [2]Hasselt University - DSI, Hasselt, Belgium; [3]Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany*

MP 381 **MassLite: An Integrated Python Platform for Single Cell Mass Spectrometry Data Pretreatment**; Zhu Zou[1]; Zhibo Yang[1]; *[1]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK*

MP 382 **Spectrum Averaging Algorithms for Increasing Mass Accuracy and Signal-to-Noise for Poorly Resolved and Low Abundance Peaks in Top-Down Proteomics**; Nicholas E. Bollis[1]; Austin V. Carr[1]; Claire Boos[1]; Lloyd M Smith[1]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, WI*

MP 383 **GlycoNetwork: A software for relating glycan expression with glycoenzyme activity**; Xavier A Holmes[1]; Michael Russelle S Alvarez[1]; Armin Oloumi[1]; Erin K. Morissette[1]; Carlito B. Lebrilla[1]; *[1]University of California Davis, Davis, CA*

MP 384 **Sensitivity analysis of isotope ratio measurements by MC-ICP-MS**; Piotr Radziński[1]; Jakub Karasiński[1]; Andrii Tupys[1]; Michał Piotr Startek[1, 2]; Anna Barbara Gambin[1]; *[1]University of Warsaw, Warsaw, Poland; [2]niversity Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany*

MP 385 **FTMStruct: a multi-source network traversal strategy to annotate lignin structure**; Rongjun Gao[1]; Jibao Liu[1]; Qinglong Fu[2]; Eunsang Kwon[3]; Manabu Fujii[1]; *[1]Tokyo*

Institute of Technology, Tokyo, Japan; [2]China University of Geosciences, Wuhan, China; [3]Tohoku University, Sendai, Japan

MP 386 **ExclusionMS: A Software Tool for Customizable Precursor Selection in Tandem Mass Spectrometry**; Patrick T Garrett[1]; Jeff Lane[1]; Christopher Adams[2]; Tharan Srikumar[2]; Jonathan R Krieger[2]; Sven Brehmer[2]; John R. Yates III[1]; *[1]Scripps Research, La Jolla, CA; [2]Bruker 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 Li[1]; Ryan Benz[1]; Harendra Guturu[1]; Iman Mohtashemi[1]; Theo Platt[1]; Serafim Batzoglou[1]; *[1]Seer Inc., Redwood City, CA*

MP 388 **Real-time AI-Driven Data Acquisition for High-Throughput Proteomics**; Soroush Hajizadeh[1, 2, 3]; Eric F Zaniewski[1]; Benedikt C Clemens[1]; 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]; *[1]MGH Cancer Center, Charlestown, MA; [2]Harvard Medical School, Boston, MA; [3]Broad Institute of MIT and Harvard, Cambridge, MA*

MP 389 **Gopher: Fast Gene Ontology Enrichment Analysis for Quantitative Proteomic Data**; Carolyn Allen[1]; Lindsay K Pino[1]; Sebastian Paez[1]; William E Fondrie[1]; *[1]Talus Bioscience, Seattle, WA*

MP 390 **A novel cloud-native pipeline enabling deep, unbiased proteomics at extreme scale**; Seth Just[1]; Andrew Nichols[1]; Jian Wang[1]; Iman Mohtashemi[1]; Theodore Platt[1]; Serafim Batzoglou[1]; *[1]Seer, Inc., Redwood City, CA*

MP 391 **Leveraging Python for Extending the Capability of MS Software Applications**; Stacey Simonoff[1]; Yongdong Wang[1]; Don Kuehl[1]; *[1]Cerno Bioscience, Las Vegas, NV*

MP 392 **Exact Formula for Positive False Discovery Rate (pFDR) Computation**; Justin Zhu[1]; Henock Deberneh[1]; Rovshan Sadygov[1]; *[1]UTMB 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 Chen[1]; Lei Xiong[1]; *[1]SCIEX, Redwood city, CA*

MP 394 **A GPU accelerated CDMS trap trajectory simulator and optimiser**; David Langridge[1]; Keith Richardson[1]; Jeff Brown[1]; Kevin Giles[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

MP 395 **Enhanced performance for triple quadrupole mass spectrometry using in-line injection S-funnel interface**; Pearl Kwantwi-Barima[1]; Isaac K. Attah[1]; Reta Birhanu Kitata[1]; Thomas L. Fillmore[1]; Richard D. Smith[1]; Yehia M. Ibrahim[1]; Tujin Shi[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

MP 396 **Orbitrap Single Ion STORI Plots for Determination of Mean Free Path and Collision Cross Section**; Michael B Lanzillotti[1]; James D Sanders[2]; Michael T Marty[2]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX; [2]The 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 Fremdling[1]; Tim K Esser[1]; Justin L P Benesch[1]; Joseph Gault[2]; Stephan Rauschenbach[1]; *[1]University of Oxford, Dept. of Chemistry, Oxford, United Kingdom; [2]Vertex Pharmaceuticals, Abingdon, United Kingdom*

MP 398 **A hybrid simulation-experimental approach for the design of mass spectrometer pumping system**; Tong Chen[1]; Mark Werlich[1]; John Nguyen[1]; *[1]Agilent 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 Lorenz[1]; Anna Kornilova[1]; Adrian MacLean[1]; Tak Shun Cheung[1]; Hamid Badiei[1]; *[1]PerkinElmer Inc., Woodbridge, ON*

MP 400 **Following Lasso Peptide Multistep Unthreading by LC-TIMS-UVPD-MS/MS**; Miguel Santos[1]; Kevin Jeanne Dit Fouque[1]; Julian Hegemann[2]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]Technische Universität Berlin, Berlin, Germany*

MP 401 **Electrical Discharges - Fundamental Concepts and Mitigation Techniques for Maximising Detector Performance**; Aditya Wakhle[1]; Antony N Jones[1]; Russell J Jurek[1]; David Whiteley[1]; Kevin L Hunter[1]; *[1]IMI Adaptas, CLYDE, Australia*

MP 402 **Implementing a Concurrent Distributed Computing Architecture for Simulation of electrostatic Ion trap with Space Charge in Simion**; Ayla Osgood[1]; Mark Osgood[1]; Robert Jackson[1]; *[1]Ashwood Labs, Wilton, NH*

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MP 404 **BSA-mediated Henry Reaction in Microdroplets**; Mengyuan Xiao[1]; Qi Wang[1]; Richard N Zare[2]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]Stanford 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 Wang[1]; *[1]Genomics Research Center, Academia Sinica, Taiwan; [2]Department of Chemistry, National Taiwan University, Taiwan; [3]Department 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 Liang[1]; Li-Wei Hsieh[1]; Huan-Cheng Chang[2]; Wen-Ping Peng[1]; *[1]National Dong Hwa University, Shoufeng, Hualien, Taiwan; [2]Academia 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 Sezgin[1]; Ian Jones[2]; Jeff Brown[3]; Michael Morris[3]; Rainer Cramer[1]; *[1]Department of Chemistry, University of Reading, Reading, United Kingdom; [2]Department of Biomedical Sciences, University of Reading, Reading, United Kingdom; [3]Waters Corporation, Stamford Ave, Altrincham Road, Wilmslow, United Kingdom*

MP 408 **Modelling and observation of complex chemical noise patterns in high-resolution mass spectrometers**; Eugene Moskovets[1]; Bogdan Budnik[2]; David H Perlman[3]; *[1]MassTech Inc, Columbia, MD; [2]Wyss Institute at Harvard, Boston, MA 02115; [3]Merck & Co., Inc., Cambridge, MA*

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MP 410 **Autonomous mass calibration of benchtop quadrupole Orbitrap™ mass spectrometers ensures continuous long-term operation and reliable drug compounds quantification**; Christian Klaas[1]; Siegrun Mohring[1]; Julia Kraegenbring[1]; Catharina Crone[1]; Claire Dauly[1]; Alexander Harder[1]; *[1]Thermo 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-Morskoy[1]; Suma Ramagiri[2]; Liulin Deng[3]; *[1]Perkin Elmer Health Sciences Inc, Hopkinton, MA; [2]PerkinElmer, Shelton , CT; [3]MOBILion Systems, Inc, Chadds Ford, PA*

MP 412 **Machine learning physicochemical properties from DMS microsolvating environments explained by SHAP analysis**; Cailum MK Stienstra[1]; Christian Ieritano[1]; Alexander Haack[1]; Scott Hopkins[1]; *[1]University of Waterloo, Waterloo, ON*

MP 413 **Chemical Transformations can Occur during DMS Separations: Lessons Learned from Beer's Bittering Compounds**; Christian Ieritano[1]; Alexander Haack[1]; Scott Hopkins[1]; *[1]University of Waterloo, Waterloo, ON*

MP 414 **Rapid Separation and Quantitation of Δ8/Δ9-THC and other isobaric cannabinoids by Differential Mobility Spectrometry**; Christian Ieritano[1]; Patrick Thomas[1]; Scott Hopkins[1]; *[1]University 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 Thurman[1]; Pratima Pathak[1]; Gordon A Anderson[2]; Alexandre A Shvartsburg[1]; *[1]Wichita State University, Wichita, KS; [2]GAA 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 Kline[1]; Michael W Belford[2]; Cornelia L Boeser[2]; Jingjing Huang[2]; David Bergen[2]; Kenneth R Durbin[3]; Joseph B Greer[3]; Graeme C McAlister[2]; Christopher Mullen[2]; Vlad Zabrouskov[2]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]Thermo Scientific, San Jose, CA; [3]Proteinacous, Evanston, IL*

MP 417 **Exploring protein N-glycosylation alterations between wild-type and mutant forms of Irisin**; Sayantani Chatterjee[1]; Joshua A. Klein[2]; Mu A[3, 4]; Quiyang Zhang[3]; Bruce M. Spiegelman[3, 4]; Joseph Zaia[1, 2]; *[1]Department of Biochemistry, Center for Biomedical Mass Spectrometry, Boston University Chobanian & Avedisian School of Medicine, Boston, MA; [2]Bioinformatics Program, Boston University, Boston, MA; [3]Dana-Farber Cancer Institute, Boston, MA; [4]Harvard 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 Finlay[1]; Allyson G. Yee[1]; Wojciech Gabryelski[1]; W. Scott Hopkins[2]; *[1]University of Guelph, Guelph, ON; [2]University of Waterloo, Waterloo, ON*

MP 419 **Exploring FAIMS gas flow settings for optimal detection of post-translational modifications using LC-MS/MS**; Rosalie Chu[1]; Chia-Feng Tsai[1]; Karl K Weitz[1]; Marina A Gritsenko[1]; Ronald J Moore[1]; Tao Liu[1]; *[1]Pacific 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 Grimes[1]; David Garbutt[1]; Theresa Evans-Nguyen[1]; *[1]University of South Florida, Tampa, FL*

MP 421 **An Automated Workflow for the Quantification of 8-Different Antidepressants using LC-MS/MS**; Ramisa Fariha[1]; Oluwanifemi D Okoh[1]; Emma Rothkopf[1]; Adam Spooner[1]; Anubhav Tripathi[1]; *[1]Brown University, Providence, RI*

MP 422 **Challenges with the Bioanalysis of Phosphate Pro-drugs and their Active Pharmaceutical Ingredients**; Kasie Fang[1]; Timothy Sikorski[1]; Zhuo Chen[1]; Clara Andonian[1]; Hermes Licea-Perez[1]; *[1]GSK, 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 Kuruc[1]; Haiyan Zheng[2]; Amenah Soherwardy[2]; Swapan Roy[1]; *[1]Biotech Support Group LLC, Monmouth Junction, NJ; [2]Rutgers 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 Naicker[1]; Claire Koenig[2]; Ana Martinez Del Val[2]; Sipho Mamputha[1]; Sindisiwe Buthelezi[1]; Ireshyn S Govender[1, 3]; Isak Gerber[1, 3]; Justin Jordaan[3]; Stoyan Stoychev[3]; Jesper Velgaard Olsen[2]; *[1]CSIR, Pretoria, South Africa; [2]Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; [3]ReSyn Biosciences, Pretoria, South Africa*

MP 428 **Miniaturization Strategies for Streamlined Drugs of Abuse Extraction prior to UHPLC-MS/MS Analysis**; Charlotte Hayes[1]; Alan Edgington[1]; Thomas Smith[1]; Lee Williams[1]; Adam Senior[1]; Helen Lodder[1]; Russell Parry[1]; Lucy Lund[1]; Zainab Khan[1]; Geoff Davies[1]; Claire Desbrow[1]; Dan Menasco[1]; *[1]Biotage GB Limited, Cardiff, United Kingdom*

MP 429 **On-Column Digest Followed By SPE Desalting For Rapid And Simplified Sample Processing Without Sample Transfer**; Heather Eastwood[1]; John D Laycock[1]; Manuel Bauer[2]; Fabian Wendt[2]; Qi Huang[1]; Shang Tsai[1]; *[1]Tecan, Baldwin Park, CA; [2]Tecan, Männedorf, Switzerland*

MP 430 **Optimisation of sample preparation for the analysis of β-Methylamino-L-alanine in complex matrices**; Siobhan J Peters[1]; Kenneth J Rogers[1]; Simon M Mitrovic[1]; David P Bishop[1]; *[1]UTS, Ultimo, Australia*

MP 431 **Determination of vedaprofen in livestock and fishery products using liquid chromatography-tandem mass spectrometry**; Bohyun Shin[1]; Chohee Jeong[1]; Sang Beom Han[1]; *[1]Department 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 Hwang[1]; Dokyung Kwon[1]; Jeongkwon Kim[1]; *[1]Chungnam 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. Twigg[1]; Stefani N. Thomas[1]; *[1]Department 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 Roof[1]; Hossein Fazelinia[1, 2]; Asif Amin Dar[3]; Hua C Ding[1]; Lynn A Spruce[1]; *[1]CHOP-Penn Proteomics Core, Philadelphia, Pennsylvania; [2]Department of Biomedical and Health Informatics, Children's Hospital of Philadelphia, Philadelphia, Pennsylvania; [3]Children's hospital of Philadelphia, Philadelphia, Pennsylvania*

MP 435 **A novel two-cycle immunoaffinity enrichment strategy to enhance assay sensitivity of biotherapeutics in tissues**; Yipei Zhang[1]; Mark G. Qian[1]; Linlin Dong[1]; *[1]Takeda 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 Miller[1]; Sara Lahsaee Little[1]; Jessica L. Nickerson[1]; Angela Giraldo[2]; Jean-François Noel[2]; Jean-Philippe Couture[2]; Hugo Gagnon[2]; *[1]Allumiqs Corporation, Halifax, NS; [2]PhenoSwitch 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 Laycock[1]; Heather Eastwood[1]; Shang Tsai[1]; Manuel Bauer[2]; Fabian Wendt[2]; John Wilson[3]; *[1]Tecan, Baldwin Park, CA; [2]Tecan, Männedorf, Switzerland; [3]ProtiFi, LLC, Farmingdale, NY*

MP 438 **Determination of atorvastatin calcium in human urine using LC-MS/MS**; Jie-ni Wang[1]; He-Hsuan Hsiao[1]; *[1]Department of Chemistry, National Chung Hsing University, Taichung, Taiwan*

MP 439 **Normalizing MS Data: Extracted Lipids from Latent Fingerprints**; Aleesa E Chua[1]; Leah Pfeifer[1]; Heather Desaire[1]; *[1]University of Kansas, Lawrence, KS*

MP 440 **High-throughput method combining mass spectrometry and machine learning for analysis of fingerprint lipids for biomarker discovery**; Madeline Isom[1]; Leah Pfeifer[1]; Eden Go[1]; Heather Desaire[1]; *[1]The 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. Solosky[1]; Iliana M. Claudio[2]; Kaylie I. Kirkwood[2]; Rebecca L Beres[1]; Michael G. Janech[3]; Frances M.D. Gulland[4]; Benjamin A. Neely[5]; Erin S. Baker[6]; *[1]University of North Carolina Chapel Hill, Chapel Hill, NC; [2]Department of Chemistry, North Carolina State University, Raleigh, NC; [3]Department of Biology, College of Charleston, Charleston, SC; [4]Wildlife Health Center, School of Veterinary Medicine, University of California, Davis, Davis, California; [5]Chemical Sciences Division, National Institute of Standards and Technology, Charleston, SC; [6]Department 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 Mehnert[1]; Kimberly C Fabijanczuk[1]; De'shovon M Shenault[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

MP 443 **Development of an offline 2D-LC lipidomics method**; Fernanda Monteiro Queiroz[1]; Adriana Zardini Buzatto[2]; Liang Li[1, 2]; *[1]University of Alberta, Edmonton, AB; [2]The 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 Marie[1]; Benoit Colsch[1]; François Fenaille[1]; *[1]Université 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 Bimpeh[1]; Kelly M Hines[1]; *[1]University of Georgia, Athens, GA*

MP 446 **Establishing an LC-HRIM-MS workflow for targeted and untargeted lipidomic analyses**; Rachel Harris[1]; Heidi Vitrac[1]; Michelle English[1]; James Atwood[1]; *[1]MOBILion 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 Spears[1]; Benjamin J Burris[2]; Abraham Kwame Badu-Tawiah[3]; *[1]the ohio state university, columbus, OH; [2]agriculture and food, columbus, Ohio; [3]The Ohio State University, Columbus, OH*

MP 448 **Electrospray ionization forms alkylated ammonium species that interfere with lipidomics analyses**; Joshua A Roberts[1]; Aleksandra Bushueva[1]; Meaghan Harley[1]; Karl V Wasslen[1]; Jeffrey C. Smith[1]; *[1]Carleton University, Ottawa, ON*

MP 449 **Functional role of ecdysteroids in awake and sleeping honey bee foragers**; Deepika Bais[1, 2]; Chhaya Patole[2]; Susanne Neupert[1]; Axel Brockmann[2]; *[1]University of Kassel, Kassel, Germany; [2]National Centre for Biological Sciences, Bengaluru, India*

MP 450 **Investigation of in situLipids from EAE Mouse Brain Tissue using Mass Spectrometry Imaging**; Rawan Serena Kassim[1]; Krista Berlin[1]; Stephan B. Bach[2]; Thomas G. Forsthuber[1]; *[1]Univeristy of Texas at San Antonio, San Antonio, TX; [2]University of Texas at San Antonio, San Antonio, TX*

MP 451 **Untargeted lipidomics of the Gemmata obscuriglobus bacterium under sterol synthesis inhibition conditions**; Franco Basile[1]; Shelby Wakefield[1]; Mitchell Helling[1]; Seifeddine Ben Tekaya[1]; Naomi Ward[2]; *[1]University of Wyoming, Laramie, WY; [2]Colorado 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 Shih[1]; Mei-Ling Cheng[1]; *[1]Chang Gung University, Taoyuan, Taiwan*

MP 453 **Fingerprinting the Unique Lipidome of Membrane Proteins Using Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry**; Jack P. Ryan[1]; Yun Zhu[2]; Melanie T. Odenkirk[3]; Arthur Laganowsky[2]; Erin S. Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Texas A&M University, College Station, TX; [3]University of Arizona, Tucson, AZ*

MP 454 **Automation of lipid extraction with Hamilton Vantage system**; Weng Wong[1]; James Joubert[1]; Jay Leone[1]; Peter Liu[1]; Wendy Sandoval[1]; Qingling Li[1]; *[1]Genentech, South San Francisco, CA*

MP 455 **Omega-6 Fatty Acid Oxidative Metabolism in Inflamed Dental Pulp**; Grace M Samenuk[1]; Ken M Hargreaves[1]; Qun Li[1]; Stephan BH Bach[2]; Zakery James[1]; *[1]University of Texas Health San Antonio, San Antonio, TX; [2]University of Texas San Antonio, San Antonio, TX*

MP 456 **Chemical and Physical Separation of Singly and Doubly Charged Lipids Within the Mass Spectrometer**; Kimberly Fabijanczuk[1]; James W. Hager[2]; Scott A. McLuckey[1]; *[1]Purdue University, West Lafayette, IN; [2]SCIEX, Concord, ON*

MP 457 **Using Lipid Exchange-Mass Spectrometry (LX-MS) to Uncover the Preferred Lipidome Environment Surrounding Membrane Proteins**; Melanie Odenkirk[1]; Guozhi Zhang[1]; Michael T Marty[1]; *[1]University of Arizona, Tucson, AZ*

MP 458 **Dual Metal Electrolysis Using a Theta Capillary for Lipid Analysis**; Annesha Sengupta[1]; Madison Edwards[1]; Xin Yan[1]; *[1]Department 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 Wang[1]; Xuejun Peng[1]; Surendar Tadi[2]; Erica Forsberg[1]; *[1]Bruker Scientific, San Jose, CA; [2]Bruker Scientific, Billerica, MA*

MP 460 **A discovery lipidomics workflow to maximize lipid identifications**; Vanessa Linke[1, 2, 3]; Agnieszka Chacińska[1, 2]; Joshua J. Coon[3]; *[1]Laboratory of Mitochondrial Biogenesis, IMol Polish Academy of Sciences, Warsaw, Poland; [2]ReMedy International Research Agenda Unit, IMol Polish Academy of Sciences, Warsaw, Poland; [3]Department 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 Agten[1]; Heiko Neuweger[2]; Dirk Valkenborg[1]; *[1]Hasselt University - DSI, Hasselt, Belgium; [2]Bruker Daltonik GmbH, Bremen, Germany*

MP 462 **Comparative lipidomic analysis of green algae Chlorella sorokinianaunder nutritional stresses**; Hector Najera-Gonzalez[1]; Claudio Cessar Barrera-Duarte[1]; Luis R. Herrera-Estrella[1]; Damar Lopez-Arredondo[1]; *[1]Texas Tech University, Lubbock, Texas*

MP 463 **High Confidence Targeted Data Mining of Untargeted High-Resolution Data for Lipids**; Sheher Banu Mohsin[1]; Mark Sartain[2]; Daniel Cuthbertson[2]; *[1]Agilent Technologies, Wood Dale, IL; [2]Agilent Technologies, Santa Clara, CA*

MP 464 **Cellular Lipidomics with C=C Specificity Enabled byAziridination**; Venus Pondevida[1]; Jiaxin Feng[1]; Xin Yan[1]; *[1]Texas A&M University, College Station, TX*

MP 465 **Aziridination-assisted mass spectrometry for nonpolar lipid analysis with isomer resolution**; Erin Hirtzel[1]; Madison E Edwards[1]; Dallas Freitas[1]; Xin Yan[1]; *[1]Texas A&M University, College Station, TX*

MP 466 **Structural Characterization and Accurate Relative Quantitation of Unsaturated Lipid Isomers Enabled by Aziridination**; Xin Yan[1]; Tingyuan Yang[1]; Shuli Tang[1]; *[1]Texas A&M University, College Station, TX*

MP 467 **Pigment profiles in microalgae extracts by electron-transfer MALDI: the analyzer's influence**; Luis Miguel Díaz[1]; Martha L Chacón-Patiño[2]; Chad R. Weisbrod[2]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia; [2]National High Magnetic Field Laboratory, Tallahassee, FL*

MP 468 **A quantitative discrimination study of recycled cashmere fibers using MALDI-TOF MS**; Shinya Koide[1]; Yuzo Yamazaki[2]; Mizuki Ikoma[1]; Aiko Yamaguchi[1]; Shinichi Ohashi[1]; *[1]Quality Evaluation Institute, BOKEN, Osaka, Japan; [2]Shimadzu Corporation, Kyoto, Japan*

MP 469 **Manufacture of 3D-printed portable spectrometer and MALDI-MS chips**; Yi-Ping Lee[1]; Ting-Hsuan Wu[1]; He-Hsuan Hsiao[1]; *[1]Department 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 Zhan[1]; Yanyi Huang[1, 2]; Guanbo Wang[1, 2]; *[1]Institute for Cell Analysis, Shenzhen Bay Laboratory, Shenzhen, China; [2]Biomedical 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 Thirukumaran[1]; Francine E. Yanchik-Slade[1]; Daniel Christensen[2]; Mohamed Boutaghou[1]; *[1]Shimadzu Scientific Instrument, Columbia, Maryland; [2]Consolidated Lab Services, Knoxville, TN*

MP 472 **MALDI mass spectrometry enables rapid metabolic profiling of cerebrospinal fluid in Parkinson's disease**; Patrik Bjärterot[1]; Theodosia Vallianatou[1]; Anna Nilsson[1]; Reza Shariatgorji[1]; Per Svenningsson[2]; Per E Andren[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Karolinska Institutet, Stockholm, Sweden*

MP 473 **Integrated machine learning-based approach to evaluate authenticity in various food matrices via MALDI-TOF-MS technology**; Reza Aalizadeh[1]; Anastasia S. Kritikou[1]; Sofia K. Drakopoulou[1]; Matthew Clabaugh[2]; Carsten Baessmann[3]; Nikolaos S. Thomaidis[1]; *[1]National and Kapodistrian University of Athens, Athens, Greece; [2]Bruker Daltonics, Billerica, MA; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

MP 474 **Advances in macromolecular materials research enabled by MALDI-TOF mass spectrometry**; Alyssa W May[1]; Liam Reilly[1]; Richard Reyes[1]; Alex Claiborne[1]; Marino Resendiz[2]; Megan Hill[1]; Chris Ackerson[1]; Eugene Y.-X. Chen[1]; Travis S Bailey[1]; *[1]Colorado State University, Fort Collins, CO; [2]University of Colorado, Denver, Denver, CO*

MP 475 **Imaging of Tissue pH by MALDI-TOF through In-Situ H/D Exchange**; Taylor A Murphree[1]; Erik Cressman[2]; Miklos Guttman[1]; *[1]University of Washington, Seattle, WA; [2]The 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-Jaimes[1]; Luis M. Díaz-Sánchez[1]; Guillermo Montoya[2]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia; [2]Universidad Icesi, Cali, Colombia*

MP 477 **Linking MALDI-FT-ICR phytoplankton pigment profiles with community taxonomy in a marine ecosystem**; Luis M. Díaz-Sánchez[1]; Martha L. Chacón-Patiño[2]; Chad R. Weisbrod[2]; Julian Franco[3]; Janet Vivas[3]; Cristian Blanco-Tirado[1]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia; [2]National High Magnetic Field Laboratory, Tallahassee, FL; [3]Marine and Coastal Research Institute, Santa Marta, Colombia*

MP 478 **Novel MALDI-TOF screening workflow for rapid detection of host response to SARS-CoV-2**; Ryan Walsh[1]; Greg Ourednik[1]; Les Edinboro[1]; *[1]SpectraPass, Las Vegas, NV*

MP 479 **MALDI-MS for the analysis of cultural heritage materials**; Signe Vahur[1]; Anu Teearu[1]; *[1]University of Tartu, Institute of Chemistry, Tartu, Estonia*

MP 480 **Improvements in Tissue Mimetic Models Using Gelatin Reinforcement and Sprayed Standards**; Andrew Bowman[1]; Junhai Yang[2]; David S. Wagner[2]; *[1]AbbVie, Inc., North Chicago, IL; [2]AbbVie Inc., North Chicago, IL*

MP 481 **Investigating the performance of (liquid) AP-MALDI when fitted to a modified DESI source**; Jeff Brown[1]; Emrys Jones[1]; Michael Morris[1]; Rainer Cramer[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]University 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 Cournut[1]; Paul Moustiez[2]; Yannick Coffinier[2]; Christine Enjalbal[1]; Claudia Bich[1]; *[1]Univ. Montpellier, CNRS, ENSCM, IBMM, UMR5247, Montpellier, France; [2]Univ. Lille, CNRS, UMR8520, IEMN, Lille, France*

MP 483 **Multi-laser induced MALDI post ionization (MALDI-2+) on a MALDI/ESI dual source**; Zhi Geng[1]; Xiaoqiang Zhang[1]; Wenjian Sun[1]; *[1]Shimadzu 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 He[1]; He-Hsuan Hsiao[1]; *[1]Department 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 Lee[1]; Ju-Ri Park[1]; Seohyun Hwang[1]; Won Suk Yang[1]; Je-Hyun Baek[1]; *[1]R&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 Choi[1]; Dong Huey Cheon[1]; Heejung Jang[1]; Won Suk Yang[1]; Je-Hyun Baek[1]; *[1]R&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 Delattre[1]; Ariadna Gonzalez[1]; Chelsea Nikula[2]; Lakshmi Nimishakavi[1]; Daniel O'Connor[1]; Melanie Bailey[3]; Josephine Bunch[1, 4]; Rory Steven[1]; *[1]National Physical Laboratory, Teddington, United Kingdom; [2]Sanofi, Boston, MA; [3]University of Surrey, Guildford, United Kingdom; [4]Imperial College, London, London, United Kingdom*

MP 488 **Mobile ESI Sprayer Head for Matrix Application and On-Tissue Derivatization in MALDI-MSI**; Andrew E Paulson[1]; Evan A Larson[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

MP 489 **Optimization of small molecule MSI by delipidation, derivatization, and instrument tuning**; Lia Ficaro[1]; Yik Siu[1]; Mark Alu[1]; Cynthia Loomis[1]; Drew R. Jones[1]; *[1]NYU Langone Health, New York, NY*

MP 490 **Optimization of MALDI-MSI for spatial visualization of key metabolites in different sorghum root architectures**; Robert K. Stanley[1]; Dusan Velickovic[1]; Kevin J Zemaitis[1]; Vimal Kumar Balasubramanian[1]; Holly M. Andrews[2]; Laura K. Meredith[2]; Margot Bezrutczyk[3]; Benjamin J. Cole[3]; Christopher R. Anderton[1]; *[1]Pacific*

Northwest National Laboratory, Richland, WA; [2]University of Arizona, Tuscon, Arizona; [3]Lawrence 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. Schultz[1]; Garrett C. McFadden[1]; Matthew M. Champion[1]; *[1]University of Notre Dame, Notre Dame, IN*

MP 492 **MALDI-TOF Mass Spectrometry: A tool for characterization of CBD Oils**; Les Edinboro[1]; Greg Ourednik[1]; Ryan Walsh[1]; *[1]SpectraPass, Las Vegas, NV*

MP 493 **Supraphysiological intravenous vitamin C administration promotes fatty acid β-oxidation and energy metabolism in humans**; Philenroza Thavrin[1]; Jaewoo Choi[1]; Ping Chen[2]; Qi Chen[2]; Jeanne Drisko[2]; Jan F. Stevens[1]; *[1]Oregon State University, Corvallis, OR; [2]University of Kansas Medical Center, Kansas City, KS*

MP 494 **Doo Dots: An investigational platform for performing Dried Fecal Spot (DFS)-based bioanalysis**; Thomas D Horvath[1]; Melinda A. Engevik[2]; Donald Chace[3]; *[1]Texas Children's Hospital - Microbiome Center, Houston, TX; [2]Medical University of South Carolina, Charleston, SC; [3]Capitainer, Stockholm, Sweden*

MP 495 **A decision tree for diagnosing and phenotyping polycystic ovarian syndrome based on serum metabolic fingerprints**; Ruimin Wang[1]; Lin Huang[2]; Kun Qian[1]; *[1]SJTU, Shanghai, China; [2]Shanghai Chest Hospital, Shanghai, China*

MP 496 **Clinical MS in practice: bias removal and research results in the multicentre SAPhIRE statin metabolism clinical trial**; Eugene Goh[1]; Lik Hang Wu[2]; Leroy S Pakkiri[2]; E Shyong Tai[2]; Jack Wei Chieh Tan[2]; Chester L. Drum[2]; *[1]NUS, SINGAPORE, Singapore; [2]National University of Singapore, Singapore, Singapore*

MP 497 **Metabolic Phenotypes Reflect Patient Sex and Injury Status: A Cross-Sectional Analysis**; Hope D Welhaven[1]; Avery H Welfley[1]; Prayag Pershad[2]; James Satalich[2]; Alexander C Vap[2]; Brian Bothner[1]; Ron K June[1]; *[1]Montana State University, Bozeman, MT; [2]Virginia Commonwealth University, Richmond, VA*

MP 498 **Quantitative analysis of Omega Fatty acids in human serum using Gas Chromatograph Mass Spectrometer**; Dr. Aseem Wagle[1]; Prashant Hase[1]; Bhaumik Trivedi[1]; Sanket Chiplunkar[1]; Durvesh Sawant[1]; Rahul Dwivedi[1]; Hemant Kesarkar[1]; Dheeraj Handique[1]; Dr. Pratap Rasam[1]; Dr. Jitendra Kelkar[1]; *[1]Shimadzu Analytical India Pvt. Ltd., Mumbai, India*

MP 499 **Highly standardized metabolomic analysis of clinical samples using triple quadruple mass spectrometry**; Chandrashekhar Honrao[1]; Masoumeh Dorrani[1]; Jifang Zhao[1]; Chen Dong[1]; Alessia Trimigno[1]; Keri Sheehan[1]; Elizabeth O'Day[1]; Jurre Kamphorst[1]; *[1]Olaris 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 Rydzak[1]; Ryan A Groves[1]; Raied Aburashed[1]; Maryam Mapar[1]; Ian A Lewis[1]; *[1]University 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 Forbes[2]; Thais de Assis Lopes[1]; Álex Aparecido Rossini Silva[3]; Juliana Goldbaum Crescente[4]; Michelle Harriz Braga[4]; Andréia de Melo Porcari[3]; Stefan Kempa[2]; Eduardo Luiz Rachid Cançado[4]; Regina Vincenzi Oliveira[1]; *[1]Federal University of São Carlos, São Carlos, Brazil; [2]Max Delbrück Center for Molecular Medicine in the Helmholtz Association, Berlin Institute for Medical Systems Biology, Berlin, Germany; [3]MS4Life Laboratory of Mass Spectrometry, Health Sciences Postgraduate Program, São Francisco University, Bragança Paulista, Brazil; [4]Institute of Tropical Medicine, Department of Gastroenterology, Faculty of Medicine FMUSP, University of São Paulo, São Paullo, Brazil*

MP 502 **Multi-class assessment of chemical exposure in dried blood spots: a pilot study**; Vinicius Verri Hernandes[1, 2]; Maximilian Zeyda[3]; Lukas Wisgrill[2, 3]; Benedikt Warth[1, 2]; *[1]Faculty of Chemistry, Department of Food Chemistry and Toxicology, University of Vienna, Währinger Straße 38, 1090, Austria; [2]Exposome Austria, Research Infrastructure and National EIRENE Hub, Vienna, Austria; [3]Department 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 Loftus[1]; Alan Barnes[1]; Emily G Armitage[1]; Elon Correa[2]; Lynne Howells[3]; Sén Takeda[4]; Wen Chung[5]; *[1]Shimadzu Corporation, Manchester, United Kingdom; [2]Liverpool John Moores University, Liverpool, United Kingdom; [3]Institute for Precision Health, The University of Leicester, Leicester, United Kingdom; [4]Department of Anatomy, Teikyo University School of Medicine, Tokyo, Japan; [5]Leicester 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 Ikeda[1]; Masatomo Takahashi[2]; Hata Kosuke[2]; Kohta Nakatani[2]; Shunsuke Aburaya[2]; Takeshi Bamba[2]; Yoshihiro Izumi[2]; *[1]Kyushu University, Fukuoka, Japan; [2]Medical Institute of Bioregulation, Fukuoka, Japan*

MP 506 **Evaluation of dried blood spot extraction strategies for untargeted metabolomics workflow**; Jiajun Lei[1]; Cara L. Sake[1]; John S. Chlystek[1]; Jonathan E. Katz[1, 2]; *[1]Lawrence J. Ellison Institute for Transformative Medicine, Los Angeles, CA; [2]University 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 Jeon[1]; Amy Lee[1]; Peter Jackson[1]; Nu Wang[1]; Andrea Liu[1]; Deborah Post[1]; Michael Leavell[1]; Mona Elbadawi[1]; *[1]Amyris, Emeryville, CA*

MP 509 **Evaluation of Red Blood Cell Depletion in Whole Blood Fractionation Workflows**; Sujatha Chilakala[1]; Cara L. Sake[1]; Ah Young Yoon[1]; Jonathan E Katz[1, 2]; *[1]Lawrence J. Ellison Institute for Transformative Medicine, Los Angeles, CA; [2]USC, Los Angeles, CA*

MP 510 **Integration of MALDI-guided Laser Capture Microdissection to Enhance Spatial Metabolomics**; Jong Hee Song[1]; Jessica K Lukowski[1]; Minsoo Son[1]; Antonia Zamacona Calderon[1]; Byoung-Kyu Cho[1]; Young Ah Goo[1]; *[1]Mass 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 Gadara[1]; Michaela Schwaiger-Haber[1]; Madelyn M. Jackstadt[1]; Madison Barr[1]; Leah P. Shriver[1]; Gary J. Patti[1]; *[1]Washington 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 Abele[1]; Etienne Doll[2]; Florian P. Bayer[3]; Chen Meng[1]; Klaus Neuhaus[4]; Siegfried Scherer[2]; Bernhard Kuster[1, 3]; Christina Ludwig[1]; *[1]BayBioMS, TUM, Freising, Germany; [2]Research Department Molecular Life Sciences, TUM, Freising, Germany; [3]Chair of Proteomics* *and Bioanalytics, TUM, Freising, Germany; [4]Core Facility Microbiome, ZIEL – Institute for Food & Health, TUM, Freising, Germany*

MP 514 **Investigating Squid-Vibrio symbiosis using MALDI-tims-qTOF-IMS**; Allyson McAtamney[1]; Denise A Ludvik[2]; Shaimaa M Aboukhatwa[3, 4]; Laura M Sanchez[1]; Mark J Mandel[2]; Terry W Moore[3]; *[1]Department of Chemistry and Biochemistry, University of California, Santa Cruz, Santa Cruz, California; [2]Department of Medical Microbiology and Immunology, University of Wisconsin-Madison, Madison, WI; [3]Department of Pharmaceutical Sciences, University of Illinois at Chicago, Chicago, IL; [4]Department of Pharmaceutical Chemistry, Tanta University, Tanta, Egypt*

MP 515 **Metaproteomics with advanced phylogenetic search space filtering in MaxQuant**; Jinqiu Xiao[1]; Shamil Urazbakhtin[1]; Juergen Cox[1]; *[1]Computational 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 Zhang[1]; Li Chen[1]; Ming Hu[1]; Jiangjiang Zhu[1, 2]; *[1]The Ohio State University, Columbus, OH; [2]The Ohio State University-Comprehensive Cancer Center, Colombus, OH*

MP 517 **Metaproteomics characterization of Svalbard permafrost active layer reveals post-thaw metabolic activities and adaptions of subsurface microbes to a warming environment**; Samantha Peters[1]; Richard J Giannone[1]; Katie Sipes[2]; Fumnanya Abuah[2]; Renxing Liang[3]; Andrey Abramov[4]; Julia Boike[5, 6]; Tatiana Vishnivetskaya[2]; Karen Lloyd[2]; Robert L Hettich[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Tennessee, Knoxville, TN; [3]Princeton University, Princeton, NJ; [4]Institute of Physiochemical and Biological Problems in Soil Science, Pushchino, Russia; [5]Alfred Wegener Institute Helmholtz-Center for Polar and Marine Research, Potsdam, Germany; [6]Humboldt-Universität zu Berlin, Berlin, Germany*

MP 518 **The role of microbial siderophores in the central nervous system and pulmonary infections**; Dominika Luptáková[1]; Rutuja Hiraji Patil[1]; Miloš Petřík[2]; Jan Hrbáček[3]; Hynek Mácha[1]; Andrea Palyzová[1]; Tereza Juříková[1]; Radim Dobiáš[4]; David Alec Stevens[5, 6]; Vladimir Havlicek[1]; *[1]Institute of Microbiology of the Czech Academy of Sciences, Prague 4, Czech Republic; [2]Institute of Molecular and Translational Medicine, Olomouc, Czech Republic; [3]Faculty Thomayer Hospital, Prague 4, Czech Republic; [4]Public Health Institute, Ostrava, Czech Republic; [5]California Institute for Medical Research, San Jose, CA; [6]Stanford University School of Medicine, Stanford, Czech Republic*

MP 519 **Automated bacterial sample preparation from Agar to MALDI target for routine bacterial identification**; Michael Douglas Nairn[1]; Philip Kirk[2]; Matthew Openshaw[1]; Oliver Severn[2]; Leah Ashley[2]; *[1]Shimadzu, Manchester, UK, Manchester, United Kingdom; [2]Singer Instruments, Roadwater, United Kingdom*

MP 520 **Comparison of Protein Extraction Methods and Data Analysis Strategies for Metaproteomic Soil Analysis**; Abigale S Mikolitis[1]; Ethan McBride[1]; Marie Kroeger[1]; Trevor Glaros[1]; Philip Mach[1]; *[1]Los Alamos National Laboratory, Los Alamos, NM*

MP 521 **Mass spectrometry-guided precision medicine: a new frontier for clinical microbiology**; Ian Lewis[1]; Daniel B. Gregson[1, 2]; Fiona Clement[1]; Ashlee Earl[3]; Yonatan Grad[4]; Hallgrimur Benediktsson[1, 2]; Bruce Walker[3]; M. Ethan McDonald[1]; *[1]University of Calgary, Calgary, AB; [2]Alberta Precision Laboratories, Calgary, AB, Canada, Calgary, AB; [3]Broad Institute of MIT and Harvard, Cambridge, MA; [4]Harvard 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 Appala[1]; Kelly M Hines[1]; *[1]University of Georgia, Athens, GA*

MP 523 **Pseudomonas aeruginosa - Rhizopus microsporus interaction: a metabolomics hunt for an antifungal treatment for Mucormycosis**; Emily C. Giedraitis[1]; Vanessa V. Phelan[1]; *[1]Department 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 Weng[1]; Christopher Suarez[1]; Karen Kalanetra[1]; Chad Masarweh[1]; David A. Mills[1]; Carlito B. Lebrilla[1]; *[1]UC Davis, Davis, CA*

MP 525 **Simplified molecular imaging analysis of excreted microbial metabolites using a benchtop MALDI-TOF system**; Sidrah Rahman[1]; Michael Douglas Nairn[2]; Rian Griffiths[3]; Tom K. Abban[4]; *[1]School of Pharmacy, University of Nottingham, Nottingham, United Kingdom; [2]Shimadzu, Manchester, UK, Manchester, United Kingdom; [3]School of Pharmacy, University of Nottingham, Nottingham, United Kingdom; [4]Shimadzu, Manchester, UK, Manchester, United Kingdom*

MP 526 **Spent media analysis and metabolic modelling of recombinant E. coli**; Pramod P Wangikar[1, 2]; Hardik Dodia[1]; Vivek Mishra[2]; Bhushan Burkul[2]; Charandatta Muddana[2]; Anant Kedia[2]; Prajval Nakrani[2]; Sneha Rana[3]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Clarity Bio Systems India Pvt Ltd, Pune, India; [3]Indian Institute of Technology, Bombay, Mumbai, India*

MP 527 **Spent amino acid analysis opens paths to improve recombinant protein production in complex media**; Hardik Dodia[1]; Vivek Mishra[2, 3]; Deepti S[1]; Pramod P Wangikar[1, 3]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Indian Institute of Technology, Bombay, Mumbai, India; [3]Clarity 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 Burguet[1]; Raphaël La Rocca[1]; Christopher Kune[1]; Alexandre Bastin[1]; Déborah Tellatin[1]; Sébastien Rigali[1]; Loïc Quinton[2]; *[1]University of Liege, Liege, Belgium; [2]University of Liège, Liège, Belgium*

MP 529 **Probability-based taxonomic profiling of microbiome samples using PepGM and Unipept**; Tanja Holstein[1, 2, 3]; Pieter Verschaffelt[2, 4]; Lennart Martens[2, 3]; Thilo Muth[5]; *[1]Bundesanstalt für Materialforschung - und Prüfung, Berlin, Germany; [2]VIB-UGent Center for Medical Biotechnology, Gent, Belgium; [3]Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; [4]Department of Applied Mathematics, Computer Science, and Statistics, Ghent University, Ghent, Belgium; [5]Bundesanstalt 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. Jamieson[1]; Eli Smart[1]; Gabriella Brown[1]; Jaewoo Choi[1]; Ryan Bradley[2]; Thomas O. Metz[3]; Jan Frederik Stevens[1]; *[1]Oregon State University, Corvallis, OR; [2]National University of Natural Medicine, Portland, Oregon; [3]PNNL, Richland, WA*

MP 531 **Using RTMS to Unravel the Microbiome Molecular Mechanisms of Carbon and Nutrient Cycling during Rewetting after Drought**; Mary S Lipton[1]; Karl K Weitz[1]; Montana L Smith[1]; James J Moran[2]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Michigan State University, East Lansing, MI*

MP 532 **Changes in the gut metaproteome of women with different body mass index status**; Gustavo Diaz[1]; Kitty Brown[1]; Amirmansoor Hakimi[2]; Corey Broeckling[1]; Jessica Prenni[3]; Mikayla A. Borton[4]; Kelly C. Wrighton[4]; *[1]Analytical Resources Core: Bioanalysis and Omics, Colorado State University, Fort Collins, CO; [2]ThermoFisher Scientific, San*

Jose, CA; [3]Department of Horticulture and Landscape Architecture, Colorado State University, Fort Collins, CO; [4]Department 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 Larson[1]; Monika Tokmina-Lukaszewska[1]; Hunter Fausset[1]; Gwendolyn Cooper[1]; Scott Spurzem[1]; Savannah Cox[1]; Rachel Spietz[1]; Brooklynn Brekke[1]; Jordan Pauley[1]; Eric Boyd[1]; Brian Bothner[1]; *[1]Montana State University, Bozeman, MT*

MP 534 **Targeted Metabolomics to unveil gut metabolite signatures identifies quinic acid as disease promoting factor in endometriosis**; Chandni Talwar[1]; Pooja Popli[1]; Satwikreddy Putluri[2]; Chandrasekhar R. Ambati[2]; Abu Hena Mostafa Kamal[2]; Ramakrishna Kommagani[1]; *[1]Department of Pathology and Immunology, Baylor College of Medicine, One Baylor Plaza, Houston, TEXAS; [2]Department 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. Neugent[1]; Neha V. Hulyalkar[1]; Philippe E. Zimmern[2]; Vladimir Shulaev[3]; Nicole J. De Nisco[1, 2]; *[1]Department of Biological Sciences, The University of Texas at Dallas, Richardson, Texas; [2]Department of Urology, The University of Texas Southwestern Medical Center, Dallas, Texas; [3]Department of Biological Sciences, The Univeristy 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 Dorfer[3]; *[1]VIB - UGent Center for Medical Biotechnology, Gent, Belgium; [2]Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; [3]Bioinformatics 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. Rajczewski[1]; Jose Alfredo Blakeley-Ruiz[2]; Matthew R. McIlvin[3]; Annaliese Meyer[3]; Tim Van Den Bossche[4]; Brian C Searle[5]; Timothy J Griffin[1]; Makoto Saito[3]; Manuel Kleiner[2]; Pratik D Jagtap[1]; *[1]University of Minnesota, Minneapolis, MN; [2]North Carolina State University, Raleigh, NC; [3]Woods Hole Oceanographic Institution, Falmouth, MA; [4]Ghent University, Gent, Belgium; [5]Ohio State University, Columbus, OH*

MP 538 **LC-MS Analysis of the Effects of Oral Contraceptives on the Human Gut Microbiome**; Danielle A Beerfas[1]; Myedith R Damba[1]; Ellen Kuang[1]; Christopher R Harrison[1]; *[1]San Diego State University, San Diego, CA*

MP 539 **Discovery and identification of a non-lethal mechanism for intercolony inhibition (“sibling rivalry”) in Marinobacter**; Ellen Kuang[1]; Heather Thorogood[1]; Mary W Carrano[1]; Erica M Forsberg[1, 2]; Carl J Carrano[1]; *[1]San Diego State University, San Diego, CA; [2]Bruker Scientific, LLC, Billerica, MA*

MP 540 **Nextgen Metaproteomics: Metaproteomics analysis using predicted deep learning library searching**; Pratik Dilip Jagtap[1]; Subina P Mehta[1]; Wassim Gabriel[2]; Andrew T. Rajczewski[1]; James Johnson[1]; Reid Wagner[1]; Mathias Wilhelm[2]; Brian C Searle[3]; Timothy J Griffin[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Computational Mass Spectrometry, Technical University of Munich, Freising, Germany; [3]The Ohio State University, Columbus, OH*

MP 541 **Temporal profiling of the extracellular proteome secreted by Escherichia coli during biofilm formation on various mannoside surfaces**; Mengfan Wang[1]; Guoting Qin[1]; Chengzhi Cai[1]; Jennifer Copeland[2]; Huamin Cai[2]; *[1]University of Houston, Houston, TX; [2]VICI 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 Li[1]; Guoting Qin[1]; Mengfan Wang[1]; Jennifer Copeland[2]; Huamin Cai[2]; Chengzhi Cai[1]; *[1]University of Houston, Houston, TX; [2]VICI Valco Instruments, Houston, TX*

MP 543 **Microbiota-Dependent Metabolomic Changes Nutritional Intervention during Pregnancy**; Emma R Guiberson[1]; Brian Defelice[2]; Josh Elias[2]; Justin L Sonnenburg[1, 2, 3]; *[1]Department of Microbiology and Immunology, Stanford University, Palo Alto, CA; [2]Chan-Zuckerberg Biohub, San Francisco, CA; [3]Center 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 Wairegi[1]; Abraham Kwame Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

MP 545 **Photoswitch-decorated nanoparticle for on-chip protein separation and mass spectrometric determination**; Tanushree Dutta[1]; Julea Vlassakis[1]; *[1]Rice University, Houston, TX*

MP 546 **High-Throughput Ultra-Low Flow LCMS platform for low sample amount proteome profiling**; Paul Jacobs[1]; Santosh Renuse[2]; Xuefei Sun[3]; Yuan Lin[3]; Jeff Op De Beeck[1]; *[1]Thermo Fisher Scientific - Belgium, Ghent, Belgium; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Sunnyvale, CA*

MP 547 **Use of microchip capillary electrophoresis – mass spectrometry for automated rapid measurement of enzyme reaction kinetics**; Gili Ben-Nissan[1]; David Morgenstern[1]; Simon Krabbe[2]; J. Will Thompson[2]; Scott Mellors[2]; Yishai Levin[1]; Michal Sharon[1]; *[1]Weizmann Institute of Science, Rehovot, Israel; [2]908 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 Rollo[1]; Adi M Kulkarni[2]; Kate Yu[2]; Guillaume Tremintin[3]; Daniele Fabris[1]; *[1]University of Connecticutt, Storrs, CT; [2]908 Devices, Inc., Boston, MA; [3]Bruker 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 Anjum[1]; Yanting Guo[1]; Zhitao Zhao[1]; Kellye A Cupp-Sutton[1]; Si Wu[1]; *[1]University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK*

MP 550 **Exploring the possibilities for Microchip SPE-CE-MS**; J. Scott Mellors[1]; J. Will Thompson[1]; Erin A. Redman[1]; *[1]908 Devices, Inc., Carrboro, NC*

MP 551 **Microfluidics: Streamlining ink identification using mass spectrometry**; Morgan Demmler[1]; Nelson R Vinueza[1, 2]; *[1]Wilson College of Textiles, NC State University, Raleigh, NC; [2]Department 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 evolutive in vitro tool to assess immunogenicity risks**; Axel Ducret[1]; Maureen Bardet[1]; Katharina Hartman[1]; Rebecca Xicluna[1]; Céline Marban-Doran[1]; *[1]Roche 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 Lamar[1]; M. Violet Lee[1]; Sylvia C Wong[1]; Peter Tran[1]; Ola Saad[1]; *[1]Genentech Inc., South San Francisco, CA*

MP 556 **Spatial Neuropeptidome Analysis of Small Neuronal Ganglia in Blue Crab Callinectes sapidus Informed by Multimodal Mass Spectrometry**; Thao Duong[1]; Ashley Phetsanthad[1]; Peng-Hsuan Huang[1]; Vu Ngoc Huong Tran[2];

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

MP 557 **Circadian neuropeptidomics for the analysis of coupling factors controlling multiscale behavioral rhythms in Drosophila melanogaster**; Susanne Neupert[1]; Deepika Bais[1]; Anna-Sophie Kuegler[1]; Anna C Schneider[1]; *[1]University of Kassel, Kassel, Germany*

MP 558 **Improving Mass Spectrometry-Based Detection and Identification of Neuropeptides in Crustacean Hemolymph Using an Anticoagulant Buffer**; Angel E. Ibarra[1]; Wenxin Wu[1]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [2]University of Wisconsin-Madison School of Pharmacy - Madison, WI, Madison, WI*

MP 559 **Worklow for rapid automated immunopeptidome profiling**; Stoyan Stoychev[1]; Justin Jordaan[2]; Terry Lim[3]; Pouya Faridi[3]; *[1]ReSyn BioSciences, Pretoria, South Africa; [2]ReSyn Biosciences, Pretoria, South Africa; [3]Monash Uniersity, Melbourne, Australia*

MP 560 **Time-of-Day Analysis of the CSF Peptidome by nanoLC-QqTOF**; Shannon D Berneche[1]; Taylor Jorgensen[1]; Wei-Chun Kao[1]; Dharmesh Parmar[2]; Martha Gillette[1, 3]; Jonathan V. Sweedler[1, 2]; *[1]Neuroscience Program, University of Illinois at Urbana-Champaign, Urbana, IL; [2]Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana and Champaign, IL; [3]Department 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 Wahle[1]; Maximilian Zwiebel[1]; Wen-Feng Zeng[1]; Patricia Skowronek[1]; Marvin Thielert[1]; Matthias Mann[1, 2]; *[1]Max-Planck-Institute for Biochemistry, Martinsried, Germany; [2]Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark*

MP 562 **An optimized biochemical and analytical workflow to unravel the human plasma peptidome**; Andreas Zellner[1]; Steffen Tiedt[2]; Chien-Yun Lee[1]; *[1]Young Investigator Group: Mass Spectrometry in Systems Neurosciences, School of Life Sciences, Technical University of Munich, Munich, Germany; [2]Institute 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]; *[1]HI-TRON, Deutsches Krebsforschungszentrum (DKFZ), Mainz, Germany; [2]Institute 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 Zhang[1]; Kyle Hoffman[1]; Sahar Rabinoviz[1]; Chao Peng[2]; Lei Xin[1]; Baozhen Shan[1]; *[1]Bioinformatics Solutions Inc, Waterloo, ON; [2]BaizhenBio Inc., shangahi, 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 Phulphagar[1]; Claudia Ctortecka[1]; Alvaro Sebastian Vaca Jacome[2]; Susan Klaeger[3]; Eva Verzani[1]; Gabrielle Hernandez[1]; Karl R Clauser[1]; Jennifer G Abelin[1]; Steven A Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Bruker Daltonics, San Jose, CA; [3]Genentech Inc, South San Francisco, CA*

MP 566 **Neuropeptidome Profiling of the Ascaris suum Body Cavity Fluid**; Wenxin Wu[1]; Ciaran McCoy[2]; Darrin McKenzie[2]; Louise Atkinson[2]; Angela Mousley[2]; Lingjun Li[1]; *[1]University of Wisconsin Madison, Madison, WI; [2]Queen'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 Pepermans[1]; *[1]University of Antwerp, Antwerpen, Belgium; [2]VITO - 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 Baker[1]; Lucy Song[1]; Charley Cai[1]; Selwyn Gu[1]; Leonard J. Foster[1]; *[1]University of British Columbia, Vancouver, BC*

MP 569 **Algorithm-assisted peptidomic diagnosis of clinical mycobacteria isolates**; Jia Fan[1]; Sudipa Maity[1]; Duran Bao[1]; Bo Ning[1]; Adrian Zelazny[2]; Tony Hu[1]; *[1]Tulane University School of Medicine, New Orleans, LA; [2]NIH/Clinical Center, Bethesda, MD*

MP 570 **Understanding Phosphotyrosine Signaling at the Single Spheroid Level**; Brian D Fries[1]; Alissa Nelson[2]; Amanda B Hummon[1]; *[1]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; [2]Cell Signaling Technology, Danvers, MA*

MP 571 **Assessing insulin signaling responses by protein phosphorylation surveillance in plasma extracellular vesicles**; Yi-Kai Liu[1]; Xiaofeng Wu[1]; Yury O. Nunez Lopez[2]; Richard E. Pratley[2]; Anton B. Iliuk[1, 3]; W. Andy Tao[1, 3]; *[1]Purdue University, WEST LAFAYETTE, IN; [2]AdventHealth, Orlando, FL; [3]Tymora Analytical Operations, West Lafayette, IN*

MP 572 **A guide to high-throughput dose-resolved phosphoproteomics to understand drug mechanism(s) of action**; Florian P Bayer[1]; Jana Zecha[1]; Matthew The[1]; Bernhard Kuster[1]; *[1]Technical University of Munich, Freising, Germany*

MP 573 **Three-dimensional construction of mouse brain protein atlas based on spatial multi-omics data**; Shuang Yang[1]; Jing Yuan[2]; Huali Shen[1]; Xiaohui Liu[1]; *[1]Fudan University, Shanghai, China; [2]HuaZhong University of Science and Technology, Wuhan, China*

MP 574 **Streamlined protein extraction and cleanup for unbiasedly exploring pan-bacterial phosphoproteomics**; Pei-Shan Wu[1]; Ting-An Chen[1]; I-Ying Lin[1]; Miao-Hsia Lin[1]; *[1]Department 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 Li[1]; Xiaolian Ning[1]; Zhoumei Zheng[1]; Siqi Li[1]; Ziyin Han[1]; Jie Liu[1]; Dongjie Wu[1]; Zhanlong Mei[1]; Jin Zi[1]; Siqi Liu[1]; *[1]BGI-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 Xavier[1]; Keith Ashman[3]; Peter G Hains[1]; Phillip J Robinson[1, 2]; *[1]Children's Medical Research Institute, Westmead, Australia; [2]University of Sydney, Sydney, Australia; [3]SCIEX, Sydney, Australia*

MP 577 **Phospho-site identification of multiply phosphorylated tau peptides in human brain**; Gunnar Brinkmalm[1]; Juan Lantero Rodriguez[1]; Elena Camporesi[1]; Laia Montoliu-Gaya[1]; Johan Gobom[1]; Ann Brinkmalm[1]; Tammaryn Lashley[2]; Henrik Zetterberg[1]; Kaj Blennow[1]; *[1]University of Gothenburg, Molndal, Sweden; [2]University College London, London, United Kingdom*

MP 578 **Improving tryptic digestion efficiency for proteomic samples by metal ion additives**; Kosuke Ogata[1]; Shunsuke Tanaka[2]; Ayana Tomioka[1]; Eisuke Kanao[1, 3]; Yasushi Ishihama[1, 3]; *[1]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; [2]Kyoto University, Kyoto, Japan; [3]National 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]; *[1]Department of Biochemistry, University of*

Colorado, Boulder, CO; [2]BioFrontiers Institute, University of Colorado, Boulder, CO

MP 580 **Phosphomatics V3: Expanding a web-based resource for online analysis of phosphoproteomics data**; Michael G Leeming[1]; Ching-Seng Ang[1]; Shuai Nie[1]; Swati Varshney[1]; Nicholas Williamson[1]; *[1]Melbourne 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 Seefried[1]; Daniel P. Zolg[1]; Tobias Schmidt[1]; Siegfried Gessulat[1]; Michael Graber[1]; Samia Ben Fredj[1]; Patroklos Samaras[1]; Markus Schneider[1]; Layla Eljagh[1]; Vishal Sukumar[1]; Pedro Navarro[2]; Kai Fritzemeier[2]; Yovany Cordero Hernandez[2]; Frank Berg[2]; Carmen Paschke[2]; David Horn[2]; Bernard Delanghe[2]; Christoph Henrich[2]; Martin Heinrich Frejno[1]; *[1]MSAID GmbH, Garching b.München, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 582 **Quantitative phosphoproteomics to identify candidate target engagement biomarkers related to efferocytosis and TAM RTK pathways**; Manuel Tzouros[1]; Emmanuelle Lezan[1]; David Avila[1]; Balazs Banfai[1]; Florian Wanke[2]; Nicolas Mercado[2]; Barbara Geering[2]; *[1]Roche Innovation Center Basel, Pharmaceutical Sciences, F. Hoffmann-La Roche, Ltd., Basel, Switzerland; [2]Roche 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 Muthukottiappan[1]; Alireza Dehghani[1]; Asisa Muchamedin[1]; Fatema Akter[1]; Mariana Eca Guimaraes De Araujo[2]; Cristina Coman[3]; Robert Ahrends[3]; Lukas Huber[2]; Volkmar Gieselmann[1]; Dominic Winter[1]; *[1]Institute for Biochemistry and Molecular Biology, Medical Faculty, Rheinische Friedrich-Wilhelms-University of Bonn, Bonn, Germany; [2]Medical University of Innsbruck, Innsbruck, Austria; [3]University 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 Roffey[1]; David W Litchfield[1]; *[1]Western 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 Marcu[1]; Bhavin Patel[2]; Jae Choi[2]; Dustin Frost[2]; Penny Jensen[2]; Amirmansoor Hakimi[3]; Kay Opperman[2]; Ryan Bomgarden[2]; Christopher M Rose[1]; *[1]Genentech Inc., South San Francisco, CA; [2]Thermo Fisher Scientific, Rockford, IL; [3]Thermo Fisher Scientific, San Jose, CA*

MP 586 **Characterizing the effects of kinase inhibitors on the phosphorylation of transcription factors using subcellular fractionation**; Andrea I Gutierrez[1]; Isabella T Whitworth[2]; Carolyn Allen[1]; William E Fondrie[1]; Daniele Canzani[1]; Lindsay K Pino[1]; Alexander J Federation[1]; *[1]Talus Bioscience, Seattle, WA; [2]University of Wisconsin-Madison, Madison, WI*

MP 587 **Multi-species Benchmarking Phospho-DIA Comparison of Commercial Sample Prep Kits**; Billy W Newton[1]; Audrick Yang[1]; Ying Zhu[1]; Guanghui Han[1]; *[1]BGI Americas, San Jose, CA*

MP 588 **Advancements in phosphopeptide elucidation is possible: permethylation via TrEnDi improves LCMS detection of phosphopeptides**; Samiksha Vij[1]; Karl Wasslen[1]; Jeffrey M Manthorpe[1]; Jeffrey C Smith[1]; *[1]Carleton University, Department of Chemistry, Ottawa, ON*

MP 589 **Characterizing Root Exudate Composition Across 19 Cover Crop Species**; Valerie Seitz; *Colorado State University, Fort Collins, CO*

MP 590 **GC-MS Profiling of Compounds Present in the Endangered Plant Ziziphus celata**; Emily Boyette[1]; Luc Alfred[1]; Sarah Arnan[1]; Toby Ellison[1]; Jenna Gutierrez[1]; Stephanie Hicks[1]; Nylla Wilder[1]; Kate Calvin[1]; *[1]South Florida State College, Avon Park, FL*

MP 591 **A Suspension Trapping-based Sample Preparation Workflow for Sensitive Plant Phosphoproteomics**; Chin-Wen Chen[1]; Chia-Feng Tsai[2]; Shu-Yu Lin[3]; Chuan-Chih Hsu[1]; *[1]Institute of Plant and Microbial Biology, Academia Sinica, Taipei city, Taiwan; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Academia Sinica Common Mass Spectrometry Facilities for Proteomics and Protein Modification Analysis, Academia Sinic, 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 Ueda[1]; Farhad Massomi-Aladizgeh[2]; M. Asaduzzaman Prodhan[3]; Mehdi Mirzaei[2]; Ghasem Hosseini Salekdeh[2]; Matthias Wissuwa[1]; Paul A. Haynes[2]; *[1]Japan International Research Center for Agricultural Sciences (JIRCAS), Tsukuba, Japan; [2]Macquarie University, North Ryde, Sydney, Australia; [3]University 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. Kilgore[1]; Anna Matthiadis[1]; Devarshi Selote[1]; Jack Wilkinson[1]; *[1]Elo Life Systems, Durham, NC*

MP 594 **Extending a Tandem Mass Spectral Library with High-Quality Reference Spectra of 11,000 Plant Metabolites**; Xiaoyu Yang[1]; Pedatsur Neta[1]; H. Martin Garraffo[1]; Yuxue Liang[1]; Yamil Simón-Manso[1]; Yi Liu[1]; Dmitrii V. Tchekhovskoi[1]; Yuri A. Mirokhin[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

MP 595 **Metabolomics Revealed the Roles of Oxylipins and Melatonin in Stomatal Immunity**; Qingyuan Xiang[1]; Craig Dufresne[2]; Sixue Chen[1, 3]; *[1]Department of Biology, Genetics Institute, University of Florida, Gainesville, FL; [2]Thermo Scientific Training Institute, West Palm Beach, Florida; [3]Department 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]; *[1]Academia Sinica, Taipei, Taiwan; [2]Academia Sinica Metabolomics Core Facility, Taipei, Taiwan*

MP 597 **Dimensionality reduction methods and GNPS for plant metabolomics ofCentella 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 Cruz[5]; Gerrad Jones[5]; Kadine Cabey[2, 6]; Ramya Viswanathan[2, 6]; Sumanaa Rajagopal[2, 6]; James Smith[7]; Amala Soumyanath[2, 6]; Jan F. Stevens[2, 3, 8]; Claudia Maier[1, 2, 3]; *[1]Department of Chemistry, Oregon State University, Corvallis, OR; [2]BENFRA Botanical Dietary Supplements Research Center, Oregon Health and Science University, Portland, OR; [3]Linus Pauling Institute, Oregon State University, Corvallis, OR; [4]Oregon Wild Harvest, Redmond, OR; [5]Biological & Ecological Engineering, Oregon State University, Corvallis, OR; [6]Department of Neurology, Oregon Health & Science University, Portland, Oregon; [7]School of Food Science & Nutrition, University of Leeds, Leeds, United Kingdom; [8]Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR*

MP 598 **From exploratory analysis to high-throughput quantitative analysis ofWithania somiferaextract 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]; *[1]Department of Chemistry, Oregon State University, Corvallis, OR; [2]BENFRA Botanical Dietary Supplements Research Center, Oregon Health and Science University, Portland, OR; [3]Linus Pauling Institute, Oregon State University, Corvallis, OR; [4]Department of Neurology,* *Oregon Health & Science University, Portland, OR; [5]Department of Neurology, Oregon Health & Science University, Portland, Oregon; [6]Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR*

MP 599 **Plant Proteomic Response to Complex Microbial Community Topsoil Inoculation**; Brandon A Saiz[1]; Linda Van Diepen[1]; Franco Basile[1]; Rachel Standish[2]; *[1]University of Wyoming, Laramie, WY; [2]Murdoch University, Perth, Australia*

MP 600 **Inside into the proteome of Chelidonium majus latex**; Joanna Gracz-Bernaciak[1]; Oliwia Mazur[1]; Natalia Kielich[1]; Michalina Krakowiak[1]; Sophia Bałdysz[1]; Martyna Węglewska[1]; Oskar Musidlak[1]; Agata Malinowska[2]; Robert Nawrot[1]; *[1]Adam Mickiewicz University in Poznan, Faculty of Biology, Department of Molecular Virology, Poznan, Poland; [2]Polish 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 Cataldi[1]; Ana Lúcia Mendes Pinheiro[1]; Felipe Garbelini Marques[1]; Alline Sekiya[1]; Fabrício Edgar De Moraes[1]; Carlos Alberto Labate[1]; *[1]ESALQ, 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]; *[1]DOE Great Lakes Bioenergy Research Center, Michigan State University, East Lansing, MI; [2]Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI; [3]Department of Plant, Soil and Microbial Sciences, Michigan State University, East Lansing, MI; [4]Department 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 Nanda[1]; Andrew Mahan[1]; Zoe Zhang[2]; Partha Chowdhury[1]; *[1]Janssen Research & Development, Spring House, PA; [2]SCIEX, Redwood city, CA*

MP 604 **Standard-Free Absolute Quantitation of Antibody Deamidation Degradation and Host Cell Proteins by Coulometric Mass Spectrometry**; Yongling Ai[1]; Harsha P. Gunawardena[2]; Xuanwen Li[3]; Yong-Ick Kim[1]; Howard D. Dewald[4]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]Janssen Research & Development, Spring House, PA; [3]Analytical Research & Development, Merck & Co., Inc., Kenilworth, NJ; [4]Ohio 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 Wong[1]; M. Violet Lee[1]; Ola Saad[1]; *[1]Genentech 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 Rivera[1]; Sergei Saveliev[1]; Michael M. Rosenblatt[1]; Ethan Strauss[1]; Matt Larsen[1]; Evan Hsu[1]; John Van Herwynen[1]; Marjeta Urh[1]; *[1]Promega Corporation, Madison, WI*

MP 608 **Peptide Mapping of a Monoclonal Antibody Using an Integrated Protein Digestion LCMS Platform (Perfinity-QTOF LCMS-9030)**; Kate (xiaomeng) Xia[1]; Evelyn H. Wang[1]; Stephen Kurzyniec[1]; Tairo Ogura[1]; Yoshiyuki Okamura[1]; Mohamed Boutaghou[1]; *[1]Shimadzu 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 Saveliev[1]; Chris Hosfield[1]; Alba Katiria González Rivera[1]; Marjeta Urh[1]; Michael M. Rosenblatt[1]; *[1]Promega 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 Aslebagh[1]; Kai Zheng[1]; *[1]CytomX Therapeutics, South San Francisco, CA*

MP 611 **Intact Mass Analysis of Biotherapeutic Stability in Tissues**; Yunan Wang[1]; Mei Han[1]; Justin Iwuagwu[1]; Fang Xie[1]; Lin Zeng[1]; Kip Conner[1]; *[1]Amgen, Inc., South San Francisco, CA*

MP 612 **Enhanced biopharmaceutical characterization using next generation multireflecting time-of-flight technology**; Guillaume Bechade[1]; Dale A Cooper-Shepherd[2]; Emma Marsden-Edwards[2]; Martin E. Palmer[2]; *[1]Waters S.A.S, Saint-Quentin, France; [2]Waters Corporation, Wilmslow, United Kingdom*

MP 613 **Characterization of carbamoylated lysine in a therapeutic recombinant protein top-down electron fragmentation**; Joaquín Barbeito[1]; Rachel Franklin[2]; Joseph Meeuwsen[2]; Mike Hare[2]; Yury Vasil'ev[2]; Joseph Beckman[2]; *[1]Xeptiva, Montevideo, Uruguay; [2]e-MSion, 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 Lafont[2]; Mathieu Dupré[2]; Norbert Zombori[2]; Alain Krick[2]; Christine Mauriac[2]; Julia Chamot-Rooke[1, 3, 4]; *[1]Institut Pasteur, Paris, France; [2]Sanofi, Chilly-Mazarin, France; [3]Université Paris Cité, Paris, France; [4]CNRS, Paris, France*

MP 615 **Characterization of Charge Variants by Ion Exchange Chromatography and Mass Spectrometry**; Yun Zhang[1]; Li-I Tsao[1]; Tiffany Hawkins[1]; Brian Woodrow[1]; *[1]MilliporeSigma, Rockville, MD*

MP 616 **"Flash Characterization" of Antibodies via Microdroplet Reactions in an Unmodified Jet Stream Source**; Michael D Knierman[1]; Jim Lau[2]; Hui Zhao[2]; Harsha P. Gunawardena[3]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Wilmington, DE; [3]Janssen 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 Batabyal[3]; Dayong Qiu[1]; Weidong Cui[1]; John Harrahy[1, 4]; Alexander R. Ivanov[2]; *[1]Amgen Inc., Cambridge, MA; [2]Northeastern University, Boston, MA; [3]Amgen, Thousand Oaks, CA; [4]Sanofi, Cambridge, MA*

MP 618 **Multi-attribute method (MAM) for biotherapeutics characterization: biosimilarity assessment, high-throughput and low-flow analytical methods applications**; Silvia Millan Martin[1]; Craig Jakes[1]; Lisa Strasser[1]; Sara Carillo[1]; Jonathan Bones[1, 2]; *[1]NIBRT, Dublin, Ireland; [2]University College Dublin, Belfield, Ireland*

MP 619 **Peptide mapping workflow for direct microchip CE-MS analysis of biopharmaceuticals**; Sara Carillo[1]; Rachel Ronan[1]; Adi M Kulkarni[2]; Erin Redman[3]; Kate Yu[2]; Jonathan Bones[1]; *[1]Characterization and Comparability Laboratory, NIBRT, Dublin, Ireland; [2]908 Devices, Inc., Boston, MA; [3]908 Devices, Inc., Carrboro, NC*

MP 620 **Mass spectrometry-based approaches to investigate allosteric modulation and biased signaling of GPCR's**; Parth Kapoor[1]; Idlir Liko[1]; Fernando Almeida[1]; Jonathan Hopper[1]; Joanna Toporowska[2]; Argyris Politis[3]; Hsin-yung Yen[4]; *[1]OMass Therapeutics, Oxford, United Kingdom; [2]King's College London, London, United Kingdom; [3]University of Manchester, Manchester, United Kingdom; [4]Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan*

MP 621 **Development of Multi-Attribute method (MAM) for heavily glycosylated protein vaccines**; Asif Shajahan[1]; Vera B. Ivleva[1]; Jason G. Gall[1]; Q. Paula Lei[1]; *[1]Vaccine*

Production Program, Vaccine Research Center, National Institutes of Health, Gaithersburg, MD

MP 622 **Novel approach to achieve high spectral quality without compromising identification for biopharma applications**; Stephane Houel[1]; Sara Carillo[2]; Craig Jakes[2]; Silvia Millán-Martín[2]; Sega Ndiaye[3]; Kevin L Schauer[1]; Jonathan Bones[2]; Shannon Eliuk[1]; *[1]ThermoFisher Scientific, San Jose, CA; [2]NIBRT, Dublin, Ireland; [3]Thermo Fisher Scientific, Courtaboeuf, France*

MP 623 **In Vivo Structural Analysis of Membrane Proteins via Hydroxyl Radical Footprinting**; James Dowell[1]; Daniel Benjamin[1]; Faraz Choudhury[1]; *[1]Immuto Scientific, Madison, WI*

MP 624 **Investigations of a Bispecific Antibody Dimerization via Hydroxyl Radical Footprinting**; Harsha Gunawardena[1]; Andrew Mahan[1]; Hirsh Nanda[1]; Daniel Benjamin[2]; *[1]JOHNSON AND JOHNSON, Spring House, PA; [2]Immuto 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 Bhattacharya[1]; Srishti Joshi[1]; Anurag Singh Rathore[1]; *[1]Indian Institute of Technology, Delhi, Delhi, India*

MP 626 **Multi-attribute monitoring ofaggregates and charge variants of monoclonal antibody through native 2D-SEC-MS-WCX-MS**; Sunil Kumar[1]; Tushar Sharad Savane[2]; Vadiraja Bhat[3]; Anurag Singh Rathore[2]; *[1]Indian Institute of Technology Delhi, New Delhi, India; [2]Indian Institute of Technology, Delhi,, New Delhi, India; [3]Agilent Technologies,, Bangalore, India*

MP 627 **A Disruptive Approach for Characterization of mAb Charge Variants by Imaged Capillary Isoelectric Focusing (icIEF)-UV/MS**; Greg Adams[1]; Hunter Walker[1]; Margo Wilson[1]; Scott Mack[2]; Maggie Ostrowski[2]; *[1]FUJIFILM Diosynth Biotechnologies USA, Morrisville, NC; [2]SCIEX, 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 Hamada[1]; Stefano Gotta[2]; Wen Jin[1]; Amy Claydon[3]; Amandine Boudreau[1]; *[1]SCIEX, concord; [2]Genedata, Basel, Switzerland; [3]Genedata, Cambridge, United Kingdom*

MP 629 **A Single Data Workflow Leveraging Middle-Down Sequencing to Validate Intact Mass Analysis Characterization of Therapeutic Antibodies**; Stephen Kok[1]; Maurizio Bronzetti[1]; Aude Tartiere[1]; Amy Claydon[2]; Arnd Brandenburg[3]; *[1]Genedata, San Francisco, CA; [2]Genedata, Cambridge, United Kingdom; [3]Genedata, 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 Savane[1]; Sunil Kumar[2]; Vadiraja Bhat[3]; Anurag Singh Rathore[1]; *[1]Indian Institute of Technology Delhi, New Delhi, India; [2]Indian Institute of Technology Delhi, New Delhi, India; [3]Agilent technologies, Bangalore, India*

MP 631 **Investigating the conformational dynamics of the interprotein calmodulin-nitric oxide synthase complex by cross-linking mass spectrometry**; Ting Jiang[1]; Guanghua Wan[1]; Haikun Zhang[1]; Eric Underbakke[2]; Changjian Feng[1]; *[1]UNM College of Pharmacy, Albuquerque, NM; [2]Roy 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 Röwer[1]; Christian Ortmann[2]; Andrei Neamtu[3]; Reham F. El-Kased[4]; Michael O. Glocker[1]; *[1]Proteome Center Rostock, Rostock, Germany; [2]Waters Corporation - TA Instruments, Eschborn, Germany; [3]TRANSCEND Centre, Regional Institute of Oncology (IRO) Iasi, Iasi, Romania; [4]The 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 Bdiri[1]; Roberto Vera Alvarez[3]; Bruce D Pascal[3]; Theodore Kamenecka[1]; Patrick R. Griffin[1, 2]; *[1]The Herbert Wertheim UF Scripps Institute for Biomedical Innovation & Technology, Jupiter, FL; [2]Skaggs Graduate School of Chemical and Biological Sciences, The Scripps Research Institute, Jupiter, FL; [3]Omics Informatics, Honolulu, HI*

MP 634 **Examining the Structure-Function Relationship of Enzymes using Temperature-Controlled Nanoelectrospray Mass Spectrometry**; Julian Alexander Harrison[1]; Adam Pruška[1]; Renato Zenobi[1]; *[1]ETH Zurich, Zurich, Switzerland*

MP 635 **Limited proteolysis-mass spectrometry (LiP-MS) enables global profiling of the effects of glycosylation on protein conformational changes**; Haiyan Lu[1]; Xudong Shi[2]; Lauren Fields[3]; Hua Zhang[1]; Danqing Wang[3]; Nathan V. Welham[2]; Lingjun Li[1]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; [3]Department 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 Plourde[1]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON*

MP 637 **Tracking the Mechanistic Origins of Irreversible Protein Unfolding**; Evelyn H MacKay-Barr[1]; Lars Konermann[1]; *[1]University of Western Ontario, London, ON*

MP 638 **Determining Collision Cross Sections Using Orbitrap Charge Detection Mass Spectrometry**; Kyle Patrick Bowen[1]; Michael Senko[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 639 **Establishing a decision tree for native mass spectrometry analysis of membrane proteins in complex membrane mimetics**; Weijing Liu[1]; Christopher Mullen[1]; Donggyun Kim[2]; Vadim Cherezov[2]; Gregory J Dodge[3]; Barbara Imperiali[3]; Hiruni S. Jayasekera[4]; Michael T Marty[4]; Rosa Viner[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of Southern California, Los Angeles, CA; [3]Massachusetts Institute of Technology, Cambridge, MA; [4]University 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 Kukačka[1]; Petr Novák[1, 2]; Petr Man[1, 2]; *[1]Institute of Microbiology of the CAS, v. v. i., Prague, Czech Republic; [2]Charles University, Faculty of science, Prague, Czech Republic; [3]Institute 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 Shvartsburg[1]; Roch Andrzejewski[2]; Andrew Entwistle[2]; Monika Gomola[2]; Patrick Knight[2]; *[1]Wichita State University, Wichita, KS; [2]Shimadzu 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 Kuo[1]; Yan Xin[1]; David Russell[1]; *[1]Texas A&M, College Station, TX*

MP 643 **Dysregulation of mitochondrial ClpP protease using orthosteric and allosteric inhibitors**; Monica M Goncalves[1]; Angelina S Kim[1]; Algirdas Velyvis[1]; Taylor Forrester[1]; Vincent Trudel[2]; Matthew Kimber[1]; Aaron Schimmer[3]; Andrei Yudin[2]; Siavash Vahidi[1]; *[1]University of Guelph, Guelph, ON; [2]University of Toronto, Toronto, ON;*

[3]Princess Margaret Cancer Centre, University Health Network, Toronto, ON

MP 644 **Cryo-EM atomic structure determination from macromolecularsamples produced by native electrospray ion beam deposition (ESIBD)**; Tim K Esser[1]; Jan Bohning[2]; Paul Fremdling[3]; Carol V Robinson[3]; Justin L. P. Benesch[3]; Lindsay Baker[3]; Tanmay A.M. Bharat[2]; Stephan Rauschenbach[4]; *[1]University of Oxford, Oxford, United Kingdom; [2]Structural Studies Division, MRC Laboratory of Molecular Biology, Cambridge, United Kingdom; [3]Oxford Univerisity, Oxford, United Kingdom; [4]University of Oxford, Dept. of Chemistry, Oxford, United Kingdom*

MP 645 **Structural interactomics and structure predictions reveal protein binding sites within disordered regions**; Julia Ruta[1]; Cong Wang[1]; Ying Zhu[1]; Pin-Lian Jiang[1]; Arne Elofsson[2, 3]; Boris Bogdanow[1]; Fan Liu[1, 4]; *[1]Department of Structural Biology, Leibniz Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; [2]Department of Biochemistry and Biophysics, Stockholm University, Stockholm, Sweden; [3]Science for Life Laboratory, Stockholm University, Solna, Sweden; [4]Charité – 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 Donor[1]; Amber Rolland[2, 3]; Takumi Takata[4]; Kirsten J Lampi[5]; James S. Prell[3]; *[1]George Fox University, Newberg, OR; [2]Utrecht University, Utrecht, Netherlands; [3]University of Oregon, Department of Chemistry and Biochemistry, Eugene, OR; [4]Kyoto University, Kyoto, Japan; [5]Oregon 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 Tonnizo[1, 3]; Marek Polák[1, 2]; Lukáš Fojtík[1, 2]; Daniel Kavan[1, 2]; Petr Man[1, 2]; Petr Novák[1, 2]; *[1]Charles University, Faculty of Science, Prague, Czech Republic; [2]BioCeV - Institute of Microbiology, Prague, Czech Republic; [3]University 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 Lin[1]; Fabia Canonica[2]; Simone Wüthrich[1]; Paolo Nanni[1]; Ralph Schlapbach[1]; *[1]Functional Genomics Center Zurich, University of Zurich & ETH Zurich, Zurich, Switzerland; [2]Department of Dermatology, University of Zurich, Zurich, Switzerland*

MP 649 **Millisecond time-resolved hydrogen/deuterium-exchange mass spectrometry at single amino acid resolution resolves conformers ofα-synuclein familial mutants**; Lindsay Cole[1]; Ulrik H Mistarz[2]; Andrew j k Williamson[3]; Ken Cook[3]; Jenny Ho[3]; Yuqi Shi[4]; Rosa Viner[4]; Jonathan J Phillips[5]; *[1]Applied Photophysics Ltd, Leatherhead, United Kingdom; [2]Thermo Fisher Scientific, Copenhagen, Denmark; [3]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [4]ThermoFisher Scientific, San Jose, CA; [5]Living 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 Panepinto[1]; Juliana Ilmain[1]; Victor Torres[1]; Beatrix Ueberheide[1]; *[1]NYU 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. James[1]; Katelynn S. Zuercher[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

MP 652 **Characterization of loading efficiency of protein nanocages with native MS and limited charge reduction**; Kevin Cheung[1]; Daniil G Ivanov[1]; Igor A Kaltashov[1]; *[1]University 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 Kit[1]; Ian K. Webb[1]; *[1]Indiana University Purdue University Indianapolis, Indianapolis, IN*

MP 654 **Insights into the Fission Yeast Rhp6, Brl1 and Brl2 Complex using Crosslinking-MS**; Enrique Arevalo[1]; Chu Thet Ywe[1]; Sara Magoun[1]; Jonathan Garcia[1]; Prakash K. Shukla[2]; Mahesh B. Chandrasekharan[2]; *[1]Spectrus, Beverly, MA; [2]Department 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 Baker[1]; Philip C Lacey[1]; Yuan Gao[1]; Benjamin J. Jones[1]; Vicki H Wysocki[1]; *[1]The 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 Sunny[1]; Yanting Guo[1]; Kellye A Cupp-Sutton[1]; Si Wu[1]; *[1]University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK*

MP 657 **Mass spectrometry-based structural investigations of S100b**; Nolan K McLaughlin[1]; Nicole D. Wagner[1]; Michael L. Gross[1, 2]; *[1]Washington University in Saint Louis, Saint Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

MP 658 **Aggregation pathways of Transthyretins: a mass spectrometry study on health-related mutants**; Liqi Fan[1]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX*

MP 659 **Monitoring MsbA Activity under Turnover Conditions**; Tianqi Zhang[1]; Jixing Lyu[1]; Arthur Laganowsky[1]; *[1]Texas A&M University, College Station, TX*

MP 660 **Enabling simultaneous photoluminescence spectroscopy and X-ray Footprinting to study protein conformation and interactions**; Sayan Gupta[1]; Line G Kristensen[1]; Brandon Russell[1]; Shawn M Costello[2]; Susan Marqusee[2]; Corie Y Ralston[1]; *[1]Lawrence Berkeley National Laboratory, Berkeley, CA; [2]University 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 Biswas[1]; Sanjyot Vinayak Shenoy[1]; Kamal Mandal[2]; Arthur Zalevsky[2]; Ayushi Verma[1]; Audrey Kishishita[2]; Andrej Sali[2]; Sanjeeva Srivastava[1, 2]; Arun P. Wiita[2]; *[1]IIT Bombay, Mumbai, India; [2]UCSF, San Francisco, CA*

MP 662 **Electrochemical Oxidation-State Switching of Heme in Cytochrome c Reveals Associated Covalent Modifications.**; Pablo Scrosati[1]; Lars Konermann[1]; *[1]Western University, London, ON*

MP 663 **Enzyme-based arginylome discovery in whole proteomes using isotopic labeling**; Zongtao Lin[1]; Joanna M Gongora[1]; Yixuan (axe) Xie[1]; Samaneh G. Kondalaji[1]; Xingyu Liu[1]; Mingzhou Zhou[1]; Faith M Robison[1]; Dongwen Lv[2]; Anna S. Kashina[3]; Michael J. Greenberg[1]; Benjamin A Garcia[1]; *[1]Washington University in St. Louis, St. Louis, MO; [2]University of Texas Health Science Center at San Antonio, San Antonio, Texas; [3]University of Pennsylvania, Philadelphia, PA*

MP 664 **Identification of 113 new histone marks by CHiMA, a tailored database search strategy**; Jinjun Gao[1]; Xinlei Sheng[1]; Jianfeng Du[1]; Di Zhang[2]; Chang Han[1]; Yue Chen[3]; Chu Wang[2]; Yingming Zhao[1]; *[1]The University of Chicago, Chicago, IL; [2]Peking University, Beijing, China; [3]University of Minnesota, Minneapolis, MN*

MP 665 **Integrating mass spectrometry and icIEF: a state of the art technology for high-resolution characterization of protein charge heterogeneity**; Teresa Kwok[1]; Mike Zhou[1]; She Lin Chan[1]; Anna Schaefer[1]; Xiaoxi Zhang[2]; Min Du[3]; *[1]Advanced Electrophoresis Solutions Ltd., Cambridge, ON; [2]Thermo Fisher Scientific, Shanghai, China; [3]Thermo Fisher Scientific, Boston, MA*

MP 666 **Engineering an enzymatic tool for chemoselective C-terminal modification**; Clara Frazier[1]; Amy Weeks[1]; *[1]Biochemistry, 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 Datta[1]; Caitlin J. Hill[1]; Nicholas P. McCurtin[1]; Rebecca A. Scheck[1]; *[1]Tufts University, Medford, MA*

MP 668 **The regulation and functions of lysine lactylome in Escherichia coli**; Hanyang Dong[1]; Jianji Zhang[1]; Kai Zhang[1]; *[1]Tianjin Medical University, Tianjin, China*

MP 669 **Utilizing SILAC Labeled Immunoglobulins for the Absolute and Relative Quantification of Glycation and Other PTMs**; Sonal Priya[1]; Ron Orlando[1]; Marla Popov[2]; *[1]University of Georgia, Athens, GA; [2]Glycoscientific, 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 Zhang[1]; Haichuan Liu[2]; Xuezhi Bi[3]; *[1]Sciex, Redwood City, CA; [2]SCIEX, Redwood city, CA; [3]Bioprocessing 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; *Sciex, Redwood City, CA*

MP 672 **Ion Mobility Separations of Largest Peptide Epimers and Intact Isomeric Proteoforms with Variant PTM Localizations**; Gayani Wijegunawardena[1]; Hayden A Thurman[1]; Francis Berthias[2]; David Williamson[3]; Haifan Wu[1]; Gabe Nagy[3]; Ole Jensen[2]; Alexandre A Shvartsburg[1]; *[1]Wichita State University, Wichita, KS; [2]Southern Denmark University, Odense, Denmark; [3]University of Utah, Salt Lake City, UT*

MP 673 **Redox proteomics of how Trx1 promotes autophagy through transnitrosylation of Atg7 during myocardial ischemia**; Narayani Nagarajan[1]; Shinichi Oka[1]; Tong Liu[1]; Hong Li[1]; Junichi Sadoshima[1]; *[1]Rutgers 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 Zhu[1]; Adrian Guthals[2]; Joseph Meeuwsen[2]; Stephen Madden[2]; Michael C. Hare[2]; Richard Cooley[3]; Joseph Beckman[2]; *[1]Oregon State University, Corvallis, OR; [2]e-MSion, Corvallis, OR; [3]Oregon State University, Corvallis*

MP 675 **Exploring multiplexing strategies for ADP-Ribosylation**; Martin Rykar[1]; Holda Awah Anagho[1]; Ivo A Hendriks[1]; Michael L Nielsen[1]; *[1]University of Copenhagen, Copenhagen, Denmark*

MP 676 **A mass spectrometric based characterization of protein aggregates isolated from a cohort of Progressive Supranuclear Palsy patients**; Maaike Beuvink[1]; Mukesh Kumar[1]; Arthur Viode[1]; Christoph N Schlaffner[1]; Kathrin Wenger[1]; Timothy Chang[2]; Michael Deture[3]; Daniel Geschwind[2]; Dennis W Dickson[3]; Hanno Steen[1]; Judith Steen[1]; *[1]Boston Childrens Hospital, Boston, MA; [2]UCLA Mednet, Los Angeles, CA; [3]Mayo Clinic, Rochester, MN*

MP 677 **Site-specific Detection of Protein S-acylation by iodoTMT Labeling and Immobilized anti-TMT Antibody Resin Enrichment**; Jian Cai[1]; Ming Song[2]; Ming Li[1]; Michael Merchant[3]; Frederick Benz[4]; Jon Klein[1, 5]; Craig McClain[2, 6, 7, 8]; *[1]Division of Nephrology and Hypertension, Department of Medicine, University of Louisville School of Medicine, Louisville, Kentucky; [2]Division of Gastroenterology, Hepatology and Nutrition, Department of Medicine, University of Louisville School of Medicine, Louisville, KY; [3]Division of Nephrology and Hypertension, Department of Medicine, University of Louisville School of Medicine, Louisville, KY; [4]Department of Pharmacology and Toxicology, University of Louisville School of Medicine, Louisville, KY; [5]Robley Rex Veterans Affairs Medical Center, Louisville, Kentucky; [6]Alcohol Research Center, University of Louisville, Louisville, KY; [7]Hepatobiology and Toxicology Center, University of Louisville, Louisville, KY; [8]Robley 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 Anderson[1]; Yun Yang[2]; Victor Tapias[2]; Hui Xu[2]; Ruchika Bhawal[1]; Qin Fu[1]; Gary E. Gibson[2]; Sheng Zhang[1]; *[1]Proteomics and Metabolomics Facility, Cornell University, Ithaca, NY; [2]Burke 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 Vanderwall[1]; Brandon Gassaway[1]; Laura Pontano Vaites[1]; David P Nusinow[2]; Donald S Kirkpatrick[2]; J. Wade Harper[1]; Steven P Gygi[1]; Edward L Huttlin[1]; *[1]Harvard Medical School, Boston, MA; [2]Interline Therapeutics, Brisbane, CA*

MP 680 **Systematic Profiling Histone Lysine Glycerylation with Chemical Proteomics Analysis**; Yi-Cheng Sin[1]; Yue Chen[1]; *[1]University of Minnesota, Minneapolis, MN*

MP 681 **Emerging role of legumain in innate immune response – potential link to anti-inflammatory effects**; Robert Vidmar[1]; Matej Vizovišek[2]; Tilen Sever[2]; Matej Kolarič[2]; Petra Matjan Štefin[2]; Georgy Mikhaylov[2]; Andreja Kozak[2]; Thomas Reinheckel[3]; Boris Turk[2]; Marko Fonović[2]; *[1]Jozef Stefan Institute, Ljubljana, Slovenia; [2]Jozef Stefan Institute, Jamova cesta 39, Slovenia; [3]Institute of Molecular Medicine, University of Freiburg, Freiburg, Germany*

MP 682 **Defining Ubiquitin Role in DNA-Protein Crosslink Repair using Mass Spectrometry**; Luke Erber[1]; Natalia Tretyakova[2]; *[1]University of Minnesota, Minneapolis, MN; [2]University of Minnesota, Twin Cities, Minneapolis, MN*

MP 683 **Development of Improved Detection Methods for Proteomic Analysis of Tyrosine Sulfation**; Cayla Rose[1]; Matt Davisson[1]; Charles Dann[1]; *[1]Indiana University Bloomington, Bloomington, IN*

MP 684 **LC-MS Identified Esterification of Glutamic Acid by Sorbitol in a Monoclonal Antibody Stability Assessment**; Bin Yu[1]; Shannon Williams[1]; Glen Young[1]; *[1]coherus bioscience, Camarillo, CA*

MP 685 **Boosting the sensitivity of electron-based fragmentation with cyclic ion mobility**; Dale A Cooper-Shepherd[1]; Emma Marsden-Edwards[1]; Darren Hewitt[1]; Jason Wildgoose[1]; Samantha Ippoliti[1]; James I. Langridge[1]; *[1]Waters 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 Li[1]; Matthew J Gaffrey[1]; Marina A Gritsenko[1]; Kiall Francis G Suazo[3]; Chia-Feng Tsai[1]; Mowei Zhou[4]; Song Feng[1]; Amy C Sims[5]; Wei-Jun Qian[1]; Tong Zhang[1]; *[1]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [2]Department of Biological Systems Engineering, Washington State University, Richland, WA; [3]Chemical Biology, Pacific Northwest National Lab, Richland, WA; [4]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; [5]Chemical 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 Wei[1]; Gordon Nicol[1]; Ping Jiang[1]; Jie Ding[1]; *[1]PPD Inc, Madison, WI*

MP 688 **Chemical proteomics and data independent acquisition enable drug target identification in Mycobacterium tuberculosis**; Dietrich Mostert[1]; Josef Braun[2]; Stephan Sieber[1]; *[1]Technical University of Munich, Munich, Germany; [2]Technical, Munich, Germany*

MP 689 **A Proteomic Investigation of Clarithromycin Resistance and Susceptibility in Mycobacterium abscessus and Mycobacterium massiliense**; Sung Hwan Yoon[1]; Ebru Selen[2]; Eva Le Run[2]; Shamira Shallom[2]; Adrian Zelazny[2]; Aleksandra Nita-Lazar[1]; *[1]NIH/NIAID, Bethesda, MD; [2]NIH/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 Branham[1]; Yulanda M. Williamson[2]; Hans C. Cooper[2]; Fabio N. Najjar[1]; John R Barr[2]; Tracie L. Williams[2]; *[1]Oak Ridge Institute for Science and Education, Atlanta, GA; [2]National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, GA*

MP 691 **Novel colistin resistance profiles of Acinetobacter nosocomialis clinical isolate, KAN02**; Hayoung Lee[1,2]; Sung Ho Yun[1]; Sang-Yeop Lee[1]; Changkyun Edmond Park[1,2]; Seung Il Kim[1]; *[1]Korea Basic Science Institute, Ochang, South Korea; [2]Korea 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 Shareef[1]; Eleanor Matthews[1]; Leroy B. Martin III[2]; Matthew E. Daly[1,3]; Christopher J. Hughes[3]; Lee Gethings[1,3,4]; Robert Plumb[2]; Simpson Angela[1]; Timothy Felton[1]; Fowler Stephen[1]; Clare Mills[1,4]; *[1]The University of Manchester NHS Foundation Trust, Manchester, United Kingdom; [2]Waters, Milford, MA; [3]Waters Corporation, Wilmslow, United Kingdom; [4]The 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 Avendaño[1]; Margarita Semis[1]; Daniel Röth[1]; Rose S. Atukunda[1]; Karine Bagramyan[1]; Lotus Lofgren[2]; Sanjeet Dadwal[1]; Jason E. Stajich[2]; Markus Kalkum[1]; *[1]City of hope, Duarte, CA; [2]University 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 Molina[1]; Daniel Röth[1]; Manuel Alfonso Patarroyo[2,3]; Markus Kalkum[1]; *[1]City of hope, Duarte, CA; [2]Fundación Instituto de Inmunología de Colombia, Bogotá, Colombia; [3]Faculty 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 Brase[1]; Sutopa Dwivedi[1]; Hager Mohamed[1]; Aykan Karabudak[1]; Patrick Romano[1]; Brian Pfister[1]; Xiaofang Huang[1]; *[1]Emergex 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 Dwivedi[1]; Richard Brase[1]; Hager Mohamed[1]; Aykan Karabudak[1]; Patrick Romano[1]; Brian Pfister[1]; Xiaofang Huang[1]; *[1]Emergex USA, Doylestown, PA*

MP 697 **Borrelia PeptideAtlas: A proteome resource for the Lyme disease community**; Helisa Wippel[1]; Jaipal P Reddy[1]; Zhi Sun[1]; David H Baxter[1]; David D. Shteynberg[1]; Melissa Caimano[2]; Robert L. Moritz[1]; *[1]Institute for Systems Biology, Seattle, WA; [2]University 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 Gotti[1]; Florence Roux-Dalvai[1]; Antoine Lacombe-Rastoll[1]; Charles Maxey[2]; Cristina Jacob[2]; Ève Bérubé[3]; Maurice Boissinot[3]; Michel G. Bergeron[3]; Neloni Wijeratne[2]; Claudia Martins[2]; Arnaud Droit[1]; *[1]Proteomics Platform and Computational Biology laboratory, CHU de Québec Université Laval Research Centre, Québec, QC; [2]Thermo Fisher Scientific, San Jose, CA; [3]Infectiology 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 Zhang[1]; Ismael A. Barreras Beltran[1]; Quynh Do[1]; Brian J. Werth[1]; Libin Xu[1]; *[1]University 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 Adcock[1]; Daniel G. Mead[1]; Franklin E. Leach III[1]; *[1]University of Georgia, Athens, GA*

MP 701 **DDA- and DIA-PASEF profiling of cross-kingdom infections reveals new mechanisms driving disease**; Brianna Ball[1]; Arjun Sukumaran[1]; Jonathan R Krieger[2]; Jennifer Geddes-McAlister[1]; *[1]University of Guelph, GUELPH, ON; [2]Bruker Ltd., Milton, ON*

MP 702 **Top-Down Proteomics Platform Enabled by Photocleavable Surfactant Azo for the Comprehensive Characterization of Endogenous Phospholamban**; Holden T Rogers[1]; David S Roberts[1]; Eli J Larson[1]; Jake A Melby[1]; Kalina J Rossler[2]; Austin V Carr[1]; Kyle A Brown[1,3]; Ying Ge[1,2,4]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Cell and Regenerative Biology, University of Wisconsin - Madison, Madison, WI; [3]Department of Surgery, University of Wisconsin-Madison, Madison, WI; [4]Human Proteomics Program, University of Wisconsin - Madison, Madison, WI*

MP 703 **Comprehensive Characterization of Protein Kinases by Native Top-Down Mass Spectrometry**; Hsin-Ju Chan[1]; Brad H. Li[2]; Boris Krichel[2]; David S. Roberts[1]; Ying Ge[1,2,3]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [3]Human 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 Causon[1]; Ihor Batruch[1]; *[1]SCIEX, 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 Goring[1]; Robert T Clubb[1]; Rachel R. Ogorzalek Loo[1]; Joseph A. Loo[1]; *[1]University of California, Los Angeles, Los Angeles, CA*

MP 706 **An integrated structural proteomics pipeline to study membrane proteins in Arabidopsis thaliana tissues**; Stephanie Thibert[1]; Jesse Wilson[1]; Vimal Balasubramanian[1]; Deseree Reid[2]; John Melchior[3,4]; Kim Hixson[5]; Tanya Winkler[1]; Roza Wojcik[2]; Aivett Bilbao[1]; Jennifer E. Kyle[3]; Mowei Zhou[1]; *[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; [2]National Security Directorate, Pacific Northwest National Laboratory, Richland, Washington; [3]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [4]Department of Pathology and Laboratory Medicine, University of Cincinnati Medical School, Cincinnati, Ohio; [5]Physical 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. Williams[1]; Dale A. Cooper-Shepherd[2]; Barbara J. Sullivan[3]; James I. Langridge[2]; Joseph A. Loo[4]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters Corporation, Milford,*

Milford, MA; [4]Department of Chemistry and Biochemistry, University of California, Los Angeles, CA

MP 708 **Capillary Zone Electrophoresis-Mass Spectrometry Reveals Histone Modification Patterns during Zebrafish Embryonic Development**; Fei Fang[1]; Qianyi Wang[1]; Liangliang Sun[1]; *[1]Michigan State University, East Lansing, MI*

MP 709 **Evaluation of Proteoform Identification by Top-Down Data-Dependent and Data-Independent Acquisition Mass Spectrometry**; Abdul Rehman Basharat[1]; Tian Xu[2]; Yong Zang[3]; Liangliang Sun[2]; Xiaowen Liu[4]; *[1]Indiana University - Purdue University Indianapolis, Indianapolis, IN; [2]Michigan State University, East Lansing, MI; [3]Indiana University School of Medicine, Indianapolis, IN; [4]Tulane 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 Melby[4]; Holden T Rogers[4]; Eli J Larson[4]; Kevin M. Buck[4]; Emily A Reasoner[4]; Hsin-Ju Chan[4]; Charlotte Uetrecht[2, 3, 5, 6]; Ying Ge[1, 4, 7]; *[1]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [2]University of Siegen, Siegen, Germany; [3]CSSB, Center for Structural Systems Biology, Hamburg, Germany; [4]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [5]German Electron Synchrotron DESY, Hamburg, Germany; [6]Leibniz Institute of Virology (LIV), Hamburg, Germany; [7]Human 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 Graham[1]; Charles F Lawlor[1]; Nicholas B Borotto[1]; *[1]University of Nevada Reno, Reno, NV*

MP 712 **Towards top-down proteomics of large proteoforms using capillary zone electrophoresis-tandem mass spectrometry**; Olivia Gordon[1]; Liangliang Sun[1]; *[1]Michigan 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 Chowdhury[1]; Yanting Guo[1]; Kellye A Cupp-Sutton[1]; Si Wu[1]; *[1]University 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 Kline[1]; Amal M Kamal[1]; Jingjing Huang[2]; David Bergen[2]; Joseph B Greer[3]; Kenneth R Durbin[3]; Graeme C McAlister[2]; Vlad Zabrouskov[2]; Christopher Mullen[2]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]Thermo Scientific, San Jose, CA; [3]Proteinaceous, Evanston, IL*

MP 715 **GeLC-FAIMS-MS Workflow for Middle-Down Proteomics**; Nobuaki Takemori[1]; Ayako Takemori[1]; Philipp T. Kaulich[2]; Ryo Konno[3]; Yusuke Kawashima[3]; Yuto Hamazaki[4]; Ayuko Hoshino[4]; Andreas Tholey[2]; *[1]Ehime University, Toon, Japan; [2]Christian-Albrechts-Universität zu Kiel, Kiel, Germany; [3]Kazusa DNA Research Institute, Kisarazu, Japan; [4]Tokyo 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 Bailey[1]; Lee K Palmer[1]; Kenneth R. Durbin[2]; William Russell[1]; *[1]University of Texas Medical Branch, Galveston, TX; [2]Proteinacous, Evanston, IL*

MP 717 **In-Source Fragmentation Data Increases Proteoform Identifications in Complex Samples**; Austin Carr[1]; Mark Scalf[1]; John G. Pavek[1]; Michael R. Shortreed[1]; Lloyd M. Smith[1]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

MP 718 **Increased Dimensional Analysis of Native Proteins via Synthetic Nanopore**; Mario Rodriguez Garcia[1]; John R. Yates III[1]; *[1]Scripps 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 Bleiholder[1]; Fanny C Liu[1]; Jusung Lee[1]; Melvin A Park[2]; Mark E Ridgeway[2]; Alina Theisen[3]; Christopher A. Wootton[4]; Stephen Fried[5]; *[1]Florida State University, Tallahassee, FL; [2]Bruker Daltonics, Billerica, MA; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [5]Johns Hopkins University, Baltimore, MD*

MP 720 **MASH Native: A Unified Solution for Native Top-Down Proteomics Data Processing**; Sean J. McIlwain[1]; Eli J. Larson[1]; Melissa R. Pergande[1]; Michelle E. Moss[1]; Kalina J. Rossler[1]; R. Kent Wenger[1]; Boris Krichel[1, 2]; Harini Josyer[1]; Jake A. Melby[1]; David S Roberts[1]; Kyndalanne A. Pike[1]; Zhouxin Shi[1]; Hsin-Ju Chan[1]; Bridget Knight[1]; Holden T. Rogers[1]; Kyle A. Brown[1]; Irene M. Ong[1]; Kyowon Jeong[3]; Michael T. Marty[4]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Siegen, Siegen, Germany; [3]University of Tübingen, Tübingen, Germany; [4]University of Arizona, Tucson, AZ*

MP 721 **Analysis of intact protein assemblies directly from living yeast colonies by native LESA mass spectrometry**; Yuying Du[1]; Robin C. May[1]; Helen J. Cooper[1]; *[1]University 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 Winnik[1]; William Padgett[1]; Emily M Pitzer[1]; David W Herr[1]; *[1]US EPA, Research Triangle Park, NC*

MP 723 **AbsoluteQuantitation of Peptides and Proteins AfterDerivatization byCoulometric Mass Spectrometry**; Praneeth Ivan Joel Fnu[1]; Md Tanim-Al-Hassan[1]; Yongling Ai[1]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ*

MP 724 **APEX Labeling and LC-MS/MS Analysis for Exploring the Proximity Proteome of YY1**; Zhongwen Cao[1]; Yenyu Yang[1]; Yinsheng Wang[1]; *[1]900 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-Castator[1]; Paolo Manzanillo[1]; Daryl Bulloch[1]; Han-Yin Yang[1]; David Chow[1]; Aman Makaju[2]; Bradford Gibson[1]; *[1]Amgen, South San Francisco, CA; [2]Amgen, Thousand Oaks, CA*

MP 726 **Solution-stabilized TMT & TMTpro reagents in 96-well plates for high-throughput sample processing**; Dustin Frost[1]; Ryan Bomgarden[1]; *[1]Thermo Fisher Scientific, Rockford, IL*

MP 727 **14-plex DeAla Isobaric Tags for High-Throughput Quantitative Proteomics**; Peng-Kai Liu[1]; Ting-Jia Gu[2]; Danqing Wang[3]; Lingjun Li[1, 2, 3]; *[1]Biophysics Graduate Program, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

MP 728 **Deciphering phytocannabinoid pharmacological effects using C. elegans, proteomics and bioinformatics.**; Fatma Boujenoui[1]; Jennifer Ben Salem[1]; Bruno Nkambeu[1]; Francis Beaudry[1]; *[1]Universite de Montreal, St-Hyacinthe, QC*

MP 729 **Determination of vanilloid targets in Caenorhabditis elegansusing Thermal proteome profiling**; Bruno Nkambeu[1]; Jennifer Ben Salem[1]; Francis Beaudry[1]; *[1]Universite de Montreal, St-Hyacinthe, QC*

MP 730 **Systematic investigation of the N-terminal effect on protein stability**; Zeyu Wang[1]; Senhan Xu[1]; Kejun Yin[1]; Xing Xu[1]; Ronghu Wu[1]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA*

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 Kraegenbring[1]; Pedro Navarro[1]; Tabiwang N. Arrey[1]; Eduard Denisov[1]; Hamish Stewart[1]; Jeff Op De Beeck[2]; Nicolaie Eugen Damoc[1]; *[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 Sun[1]; Zhiping Wu[1]; Junmin Peng[1]; *[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 Deghghani[1]; Carmen Schoor[1]; Markus Gödderz[1]; Nur Cengiz[1]; Shiva Ahmadi[1]; Ramesh Sharma[1]; Karin Schork[2, 3]; Martin Eisennacher[2, 3]; Volkmar Gieselmann[1]; Dominic Winter[1]; *[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. Tressler[1]; Rahul A. Bharadwaj[2]; Kristine Glunde[1]; Daniel Weinberger[2]; Robert N. Cole[1]; *[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 Shen[2]; Shihan Huo[2]; Sailee Rasam[2]; Min Ma[1]; 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 Martin[2]; Gary Bradshaw[2]; Robyn J Eisert[2]; Stephen C Blacklow[2]; *[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 Wang[2]; Yinsheng Wang[2]; *[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 Qi[1]; Lin Li[1]; Yinsheng Wang[1]; *[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 Zhang[2]; Ginny Xiaohe Li[3]; Fengchao Yu[3]; Felipe Da Veiga Leprevost[3]; Ralf B Schittenhelm[2]; 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 Tu[1]; Asik Didar[1]; Jaime Goldfuss[1]; Scott J. Jacobia[1]; Andrew M. Campbell[1]; *[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 Willard[1]; *[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

Ambient Ionization: Fundamentals and Instrumentation..001-015
Antibodies & Antibody Drug Conjugates I................016-041
Artificial Intelligence in MS Instrumentation and Applications...042-062
Biomarkers: Discovery II 063-087
Biomarkers: Quantitative Analysis II........................088-111
Cancer Research II 112-135
Clinical Analysis II 136-166
Covalent Labeling and Chemical Crosslinking II......167-193
Drug Discovery: Qualitative and Quantitative Analysis II.............................194-219
Environmental: General I..220-242
Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements I................243-263
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Fundamentals: Unconventional Approaches in MS..266-279
Glycoproteins II..280-312
Imaging MS: Method Development II 313-339
Imaging: Spatially-Resolved Omics I.......................340-359
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Proteins: General and Membrane............................577-592
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Proteomics: Clinical Applications............................621-652
Proteomics: Intact Proteins and Top Down Analysis II...............................653-674
Proteomics: Quantitative II 675-693
Proteomics: Tissue...694-713
Synthetic Polymers 714-725
Toxicology..726-733

TP 001 **Single Fiber Quantitation of Solid-Phase Microextraction Samples with Five-shot Direct Analysis**; G. Asher Newsome[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**; Motoshi Sakakura[1]; Teruhisa Shiota[1]; [1]*AMR Inc., Meguro-Ku, Japan*

TP 003 **The Role of Ion Suppression in Secondary Electrospray Ionization-Mass Spectrometry**; Cedric Wuethrich[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**; Shun Kumano[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**; Adriana Arigò[1]; Giovanna Nevola[1]; Giorgio Famiglini[1]; Pierangela Palma[1, 2]; Achille Cappiello[1, 2]; [1]*UNIVERSITY OF URBINO CARLO BO, URBINO, Italy;* [2]*Vancouver Island University, Nanaimo, BC*

TP 006 **Infrared Matrix-Assisted Laser Desorption Electrospray Ionization with a Heated Electrospray Emitter**; Kevan T. Knizner[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**; Wei Zhou[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**; Zhichang Yang[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** ; Dmytro S Kulyk[1]; Taghi Sahraeian[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)**; Haidy Metwally[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**; Jian Yu[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)**; Julia McPhail[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**; Igor Popov[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**;

James A Richardson[1]; Christopher J Taylor[1]; Andre Venter[1]; *[1]Western Michigan University, Kalamazoo, MI*

TP 015 **Integrating the MasSpec Pen Technology with a Time-of-Flight Mass Spectrometer for Direct Tissue Analysis**; Charles A. Wolfe[1]; Michael F. Keating[1, 2]; Viktor Zseller[3]; Tamas Karancs[3]; Steven Pringle[3]; Justin Wiseman[4]; Mike Morris[3]; Livia S. Eberlin[1]; *[1]Department of Surgery, Baylor College of Medicine, Houston, Texas; [2]The University of Texas at Austin, Austin, TX; [3]Waters Corporation, Wilmslow, United Kingdom; [4]MS Pen Technologies Inc., Houston, Texas*

TP 016 **High-Throughput Purification, Reduction and SEC-MS Glycoprofiling of a Therapeutic Monoclonal Antibody**; Stephan Altmaier[1]; Uma Sreenivasan[2]; Kevin Ray[3]; *[1]Merck KGaA, Darmstadt, Germany; [2]MilliporeSigma, Round Rock, TX; [3]MilliporeSigma, St. Louis, MO*

TP 017 **Proteomic analysis reveals insights into the mechanism of intra-CORK approach for increasing therapeutic window of immunocytokines**; Ettore Gilardoni[1]; Domenico Ravazza[1]; Giulia Rotta[1]; Sheila Dakhel[1]; Dario Neri[2, 3]; *[1]Philochem AG, Otelfingen, Switzerland; [2]ETH Zurich, Zurich, Switzerland; [3]Philogen 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 Rijswijck[1]; Albert Bondt[1]; Naomi De Kat[1]; Jonathan Sjögren[2]; Rolf Lood[2]; Albert J.R. Heck[1]; *[1]Utrecht University, Utrecht, Netherlands; [2]Genovis AB, Lund, Sweden*

TP 019 **Characterization of therapeutic antibody charge variants in drug development by microfluidic native capillary electrophoresis-mass spectrometry**; Zhijie Wu[1]; Haibo Qiu[1]; Ning Li[1]; *[1]Regeneron 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 Zhang[1]; Sensen Chen[1]; Christof Mitterer[2]; Min Du[3]; Ken Cook[4]; *[1]ThermoFisher Scientific, Shanghai, China; [2]Thermo Fisher Scientific, Langerwehe, Germany; [3]Thermo Fisher Scientific, Boston, MA; [4]Thermo 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 Eysberg[1]; Jonathan Bones[2]; Ken Cook[3]; Tomos E. Morgan[2]; Jean-Pierre Chervet[4]; *[1]Antec Scientific, Bostson, MA 02108; [2]NIBRT, Dublin, Ireland; [3]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [4]Antec 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 Adhikari[1]; Minghao Sun[2]; Eric Ma[2]; William R. Mylott Jr. [2]; Shawn Harriman[3]; Jan Pinkas[3]; Elizabeth Shaheen[3]; Feng Yin[3]; *[1]Pyxis Oncology, Cambridge, MA; [2]PPD, Richmond, VA; [3]Pyxis Oncology, Cambridge*

TP 023 **Novel icIEF-based fractionation of therapeutic antibody charge variant for LC-MS characterization**; Xiaojing Shen[1]; Philip Chao[1]; Cheng Zhou[1]; Kefei Wang[1]; Faidh Hana[2]; Zhaohui Fan[2]; Amr Ali[2]; Jian He[2]; Dave Ouellette[2]; Roland Wang[1]; Jessica Dermody[1]; *[1]ProteinSimple, a brand of Bio-techne.com, San Jose, CA; [2]AbbVie 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 Hare[1]; Adrian Guthals[1]; Joseph S Beckman[1, 2]; *[1]e-MSion, Corvallis, OR; [2]Oregon State University, Corvallis*

TP 025 **Ion Mobility-Mass Spectrometry and Collision Induced Unfolding of Chemically Modified Antibody Oligomers**; Nicole A Rivera-Fuentes[1]; Brandon T Ruotolo[2]; *[1]University of Micihigan, Ann Arbor, MI; [2]University 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 Carillo[1]; Florian Fuessl[1]; Silvia Millan Martin[1]; Shanhua Lin[2]; Jonathan Bones[1, 3]; *[1]NIBRT, Dublin, Ireland; [2]Thermo Fisher Scientific, Sunnyvale, CA; [3]School 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 Gould[1]; Jake Ocque[2]; Robin Difrancesco[2]; Qing Ma[2]; Raymond Cha[2]; Gene Morse[2]; Troy D. Wood[1]; *[1]Department of Chemistry, University at Buffalo, Buffalo, NY; [2]Department of Pharmacy Practice School of Pharmacy and Pharmaceutical sciences, University at Buffalo, Buffalo, NY*

TP 028 **Multiplexed Bioanalysis ofVariousAntibody–Drug Conjugates (ADCs)in Cynomolgus Monkey Plasmawith Using Immunoaffinity LC-MS/MS**; Eric W. Ma[1]; Minghao Sun[1]; William R. Mylott Jr. [1]; David Roos[2]; *[1]PPD, Richmond, VA; [2]Boehringer Ingelheim, Ridgefield, CT*

TP 029 **Unambiguous Identification and Localization of Isoaspartic Acid in Therapeutic Proteins by Optimized Enzymatic Digestion and Electron Transfer Dissociation**; Lidong He[1]; Jason L. Richardson[1]; Zhongqi Zhang[1]; Les Miranda[1]; Suminda Hapuarachchi[1]; Jun Zhang[1]; Jiu-Li Song[1]; *[1]Amgen, Thousand Oaks, CA*

TP 030 **Polyclonal antibody epitope mapping at single amino acid resolution for pregnancy malaria vaccine design**; Santosh A Misal[1]; Robert Morrison[2]; Jonathan Renn[2]; Yai Doritchamou[2]; Martin Burkhardt[2]; Alassane Dicko[3]; Patrick Duffy[2]; Michal Fried[1]; *[1]Molecular 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; [2]Pathogenesis 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; [3]Malaria 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 Fernandes[1]; St. John Skilton[1]; Marshall Bern[1]; Krisztina Radi[1]; Andreas Nägeli[2]; Sabrina Forni[1]; *[1]Protein Metrics, LLC, Cupertino, CA; [2]Genovis AB, Lund, Sweden*

TP 032 **Zero False Positives in Multi-Attribute Method New Peak Detection with a Statistics Guided Approach**; Qinjingwen Cao[1]; John Guan[1]; Delia Li[1]; Jennifer Zhang[1]; Riley Togashi[1]; Elizabeth Johnson[1]; Jia Guo[1]; Peilu Liu[1]; Lance Cadang[1]; Monica Sadek[1]; Feng Yang[1]; *[1]Genentech, 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 Bishop[1]; John J. Correia[1]; *[1]University 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 Woodall[1]; Christy A Thomson[2]; Thomas M Dillon[1]; Arnold McAuley[1]; Pavel Bondarenko[1]; *[1]Amgen Inc, Thousand Oaks, CA; [2]Amgen 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*

TP 036 **Facilitating LC-MS Analysis of Fusion Protein Therapeutics by Enzymatic Hydrolysis of Flexible Linkers**; Andreas Naegeli[1]; Magdalena Widgren-Sandberg[1]; Maria Nordgren[1]; Camilla Sivertsson[2]; John Lindsay[2]; Rikke Rytter[1]; *[1]Genovis AB, Lund, Sweden; [2]Genovis 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 Srzentic[1]; Angela Criscuolo[2]; Kai Scheffler[2]; Nicolaie Eugen Damoc[2]; *[1]ThermoFisher Scientific, Basel, Switzerland; [2]Thermo Fisher Scientific, Bremen, Germany*

TP 038 **Super-immunity by pan-sarbecovirus nanobodies**; Yufei Xiang[1]; Wei Huang[2]; Hejun Liu[3]; Zhe Sang[4]; Sham Nambulli[5]; Jérôme Tubiana[6, 7]; Paul Duprex[5]; Dina Schneidman-Duhovny[7]; Ian A. Wilson[3]; Derek J. Taylor[2]; Yi Shi[4]; *[1]Icahn School of Medicine at Mount Sinai, New York, NY; [2]Case Western Reserve University, Cleveland, OH; [3]The Scripps Research Institute, La Jolla, CA; [4]Icahn School of Medicine at Mt Sinai, New York, United States, NY; [5]University of Pittsburgh, Pittsburgh, PA; [6]Tel Aviv University, Tel Aviv, Israel; [7]The 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 Peng[1]; Joost Snijder[1]; Maartje Huijbers[2]; Laurent Paardekooper[2]; Dana L.E. Vergoossen[2]; *[1]University Utrecht, UTRECHT, Netherlands; [2]Leiden Univeristy Medical Centre LUMC, Leiden, Netherlands*

TP 041 **Delineating the epitope diversity of recombinant monoclonal antibodies isolated from Alpaca polyclonal mixture with HDX-MS**; Dominic Narang[1]; Thierry Le Bihan[2]; Teresa Nunez De Villavicencio Diaz[1]; Bin Ma[1]; Jennifer Crha[1]; *[1]Rapid Novor Inc., Kitchener, ON; [2]Rapid Novor Inc, Kitchener*

TP 042 **MALDI-TOF Mass Spectrometry with Machine Learning for High-Throughput Screening of Raw Milk for Evidence of Mastitis**; Jon Thompson[1]; Savana Everhart[1]; Sumon Sarkar[1]; Beth Clayton[2]; *[1]Texas Tech University, Amarillo, TX; [2]Texas Dairy Herd Improvement Association, Canyon, Texas*

TP 043 **Diving deeper with depthcharge: A transformer deep learning framework for modeling mass spectrometry data**; William E Fondrie[1]; Wout Bittremieux[2]; Melih Yilmaz[3]; William S Noble[3]; *[1]Talus Bioscience, Seattle, WA; [2]University of Antwerp, Antwerpen, Belgium; [3]University of Washington, Seattle, WA*

TP 044 **Mapping Competitive Activity Based Protein Profiling Data to AlphaFold2 Models**; Adam L Borne[1]; Yusuf Adeshina[1]; Natalia Zaliznyak[1]; Luca Naef[1]; Zachary Carpenter[1]; *[1]VantAI, New York, NY*

TP 045 **GlycoNovo: Deep learning based framework for N-linked glycan DeNovo sequencing**; Qianqiu Zhang[1]; Zeping Mao[1]; Weiping Sun[2]; Xiyue Zhang[2]; Ngoc Hieu Tran[1]; Xin Lei[2]; Baozhen Shan[2]; Ming Li[1]; *[1]University of Waterloo, Waterloo, ON; [2]Bioinformatics 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 Cai[1]; Zainab Noor[1]; Adel T Aref[1]; Emma L Boys[1]; Dylan Xavier[1]; Natasha Lucas[1]; Steven G Williams[1]; Jennifer M Koh[1]; Erin Sykes[1]; Rebecca C Poulos[1]; Peter G Hains[1]; Phillip J Robinson[1]; Rosemary Balleine[2]; Roger R Reddel[1]; Qing Zhong[1]; *[1]ProCan®, Children's Medical Research Institute, Faculty of Medicine and Health, The University of Sydney, Westmead, Australia; [2]Westmead 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 Fagerquist[1]; *[1]Produce Safety & Microbiology, Western Regional Research Center, Agricultural Research Service, USDA, Albany, CA; [2]Oak 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 Yan[1]; Qian Dong[1]; *[1]NIST, Gaithersburg, MD; [2]Georgetown University, Washington Dc, DC*

TP 049 **Transfer Learning Methods Improve Deep Fragmentation Model**; Alexandros Pachos[1]; Anna Susmelj[1]; Oliver M Bernhardt[1]; An-phi Nguyen[1]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Zurich, Switzerland*

TP 050 **AIMsPeak: a Convolutional Neural Network-Based Model for Ground-Truth Liquid Chromatography/Mass Spectrometry Features Selection**; Hiu-Lok Ngan[1]; Zongwei Cai[1]; *[1]Hong Kong Baptist University, Hong Kong, China*

TP 051 **Exploring the Temporal Metabolome of "Hyperfood" Kimchi with Data-Driven Trajectory Cluster Analysis**; Ali Lotfi[1]; Alla Veselkova[2]; Alexey Melnik[1]; Kirill Veselkov[3]; Alexander Aksenov[4]; *[1]University of Connecticut, Storrs, CT; [2]Intelligify Ltd., London, United Kingdom; [3]Imperial College London, London, United Kingdom; [4]University of Connecticutt, Storrs, CT*

TP 052 **Applying Automated Machine Learning for Classification and Regression in Large-Scale Clinical Proteomics Datasets**; Amir Alavi[1]; Harendra Guturu[1]; Guhan Venkataraman[1]; Jane Lange[2]; Matthew Chang[2]; Travis Moore[2]; Khatereh Motamedchaboki[1]; Anna Halama[3]; Frank Schmidt[3]; Karsten Suhre[3]; Mark Flory[2]; Serafim Batzoglou[1]; *[1]Seer, Inc., Redwood City, CA; [2]Oregon Health & Science University, Portland, Oregon; [3]Weill Cornell Medicine - Qatar, Education City, Qatar*

TP 053 **Estimating the uncertainty of AI predictions of the Kováts retention index**; Lewis Geer[1]; Douglas Slotta[1]; *[1]NIST, Gaithersburg, MD*

TP 054 **Transfer learning to accurately predict retention times of modified peptides with DeepLC**; Robbin Bouwmeester[1]; Alireza Nameni[1, 2]; Arthur Declercq[1, 2]; Ralf Gabriels[1, 2]; Sven Degroeve[1, 2]; Lennart Martens[1, 2]; *[1]VIB-UGent Center for Medical Biotechnology, Gent, Belgium; [2]Department 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]; *[1]VIB-UGent Center for Medical Biotechnology, Gent, Belgium; [2]Department of Biomolecular Medicine, Ghent University, Ghent, Belgium*

TP 056 **Improving Identification Confidence in Suspect Screening of Consumer Products using Machine Learning**; William D Watson[1]; Kristin A Favela[1]; Jake A Janssen[1]; Michael J Hartnett[1]; Heath A Spidle[1]; Jarod N Grossman[2, 3]; Jenna Hua[2]; *[1]Southwest Research Institute, San Antonio, TX; [2]Million Marker Wellness, Inc., Berkeley, CA; [3]Agilent Technologies, Santa Clara, CA*

TP 057 **Realistic in silico generation and augmentation of mass spectrometry based proteomics data using generative adversarial networks**; Vartika Tewari[1]; Sunghyun Huh[2]; Sangtae Kim[2]; Olga Vitek[1]; *[1]Northeastern University, Boston, MA; [2]Bertis 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

Inzamam Ul Haque[1]; Debangshu Mukherjee[2]; Nikolay Borodinov[2]; Sylwia Stopka[3]; Nathalie Agar[3, 4, 5]; Jacob Hinkle[2]; Olga S. Ovchinnikova[1, 2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]Brigham and Women's Hospital, Boston, MA; [4]Harvard Medical School, Boston, MA; [5]Dana-Farber Cancer Institute, Boston, MA*

TP 059 **Semi-supervised Metric learning for universal representation of tandem mass spectra**; Kaiyuan Liu[1]; Haixu Tang[1]; *[1]Indiana University Bloomington, Bloomington, IN*

TP 060 **Predicting tandem mass spectra of long peptides using fully convolutional networks**; Kaiyuan Liu[1]; Zhu Rui[1]; Haixu Tang[1]; *[1]Indiana 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 Abramchuk[1]; Yun-En Chung[1]; Alona Petrova[1]; Christopher Adams[2]; Jonathan R Krieger[3]; Tharan Srikumar[3]; Mathieu Lavallée-Adam[1]; *[1]University of Ottawa, Ottawa, ON; [2]Bruker Scientific LLC, San Jose, CA; [3]Bruker Ltd., Milton, ON*

TP 062 **Automating GC/MS peak integration using Machine Learning Modelling for maximizing throughput, quality and enhancing consistency**; Thomas Bispham[1]; Tamas King[2]; Winnie Chau[2]; Steve Prutzman[1]; *[1]Agilent Technologies, Cedar Creek, TX; [2]Agilent Technologies, Inc, Hong Kong, Hong Kong*

TP 063 **Comparative Analysis of Protein Folding Stability-Based Profiling Methods for the Characterization of Breast Cancer**; Morgan Bailey[1]; Hyejin Park[1]; Michael C. Fitzgerald[1]; *[1]Duke 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 Kell[1]; Sonali Mishra[1]; Toloo Taghian[2]; Heather L Gray-Edwards[2]; Daniel S Ory[3]; Xuntian Jiang[4]; *[1]Washington University School of Medicine, Saint Louis, MO; [2]University of Massachusetts Medical School, Worcester, MA; [3]Casma Therapeutics, Cambridge, MA; [4]Washington 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 Sasaki[1]; Takeo Kamakura[1]; Yuanqing Ye[2]; Satya Saxena[2]; Viswanath Devanarayan[2]; Pallavi Sachdev[2]; Kanta Horie[2]; *[1]Eisai Co., Ltd., Tsukuba-shi, Japan; [2]Eisai Inc., Nutley, NJ*

TP 067 **High-performance serum metabolic fingerprints encode breast cancer**; Yida Huang[1]; Kun Qian[2]; *[1]Shanghai Jiao Tong University, Shanghai, China; [2]Shanghai Jiao Tong University, Shanghai, China*

TP 068 **Multi-omic landscapes of Nasopharyngeal Carcinoma reveal patterns associated with induction chemotherapy response**; Dongxue Wang[1]; Yingqin Li[2]; Xianfeng Shao[1]; Chunxian Ou[2]; Jun Ma[2]; Fuchu He[1]; *[1]Beijing Proteome Research Center, National Center for Protein Sciences, Beijing, China; [2]Sun Yat-Sen University Cancer Center, guangzhou, China*

TP 069 **Energy Depletion and Metabolic Alterations in Cellular Model of Fabry Disease**; Ryan W. Pearce[1]; Jillian Kodger[1]; Igor Radzikh[1]; Yana I Sandlers[1]; *[1]Cleveland 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 Aguilar[1]; Mali Cosden[1]; Lei Ma[1]; Jacob Marcus[1]; Robert Drolet[1]; Nathan Hatcher[1]; *[1]Merck & 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 Musah[1]; Allix M. Coon[1]; Gavin Setzen[2]; *[1]University at Albany-SUNY, Albany, NY; [2]Albany 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 Do[1]; Husam Kafeenah[1]; Shu-Hui Chen[1]; *[1]National Cheng Kung University, Tainan, Taiwan*

TP 073 **Determination ofgangliosides in urine of patients suffering from diabetic kidney disease by high resolution tandem mass spectrometry**; Raluca Ica[1]; Anca Suteanu-Simulescu[2]; Mirela Sarbu[1]; Ligia Petrica[2]; Alina D. Zamfir[1, 3]; *[1]Department of Condensed Matter, National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; [2]Department of Internal Medicine II, Division of Nephrology, "Victor Babes" University of Medicine and Pharmacy, Timisoara, Romania; [3]Department 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 Hoegl[1]; Marie Louise Nautrup Therkelsen[1]; Mikkel Parsberg Werge[2]; Elias Badal Rashou[2]; Mira Thing[2]; Liv Eline Bjørge Hetland[2]; Anders Ellekær Junker[2]; Reza Serizawa[3]; Mogens Vyberg[3, 4]; Christian Toft Madsen[1]; Elisabeth Douglas Galsgaard[1]; Lise Lotte Gluud[2, 5]; Mads Grønborg[1]; *[1]Research & Early Development, Novo Nordisk A/S, Maaloev, Denmark; [2]Gastro Unit, Copenhagen University Hospital, Hvidovre, Denmark; [3]Department of Pathology, Copenhagen University Hospital Hvidovre, Hvidovre, Denmark; [4]Center for RNA medicine, Aalborg University Copenhagen, Copenhagen, Denmark; [5]Department 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 Wachter[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University 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 Lee[1]; Christine Neville[2]; Ting Huang[1]; Mitchell Rechtzigel[3]; Alex Rosa Campos[4]; Khatereh Motamedchaboki[1]; Daniel Hornburg[1]; Jill Weimer[2, 3]; Jon Brudvig[2, 3]; *[1]Seer, Inc., Redwood City, CA; [2]Amicus Theraputics, Philadelphia, Pennsylvania; [3]Pediatrics and Rare Disease Group, Sanford Research, Sioux Falls, South Dakota; [4]Sanford Burnham Prebys, San Diego, California*

TP 077 **Proteoform Detection in Deep Plasma Proteomics through Peptide Expression Correlation**; Yingxiang Huang[1]; Jian Wang[1]; Alexey Stukalov[1]; Ting Huang[1]; Margaret Donovan[1]; Daniel Hornburg[1]; Asim Siddiqui[1]; Anna Halama[2, 3]; Frank Schmidt[4, 5]; Karsten Suhre[2, 3]; Serafim Batzoglou[1]; *[1]Seer Inc., Redwood City, CA; [2]Bioinformatics Core, Weill Cornell Medicine-Qatar, Education City, Qatar; [3]Department of Biophysics and Physiology, Weill Cornell Medicine, New York, NY; [4]Proteomics Core, Weill Cornell Medicine-Qatar, Education City, Qatar; [5]Department 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 Rana[1]; Pramod P Wangikar[1, 2]; Vivek Mishra[1, 2]; Bhushan Burkul[2]; Prajval Nakrani[2]; Rakesh Kumar Sahay[3]; Lakshman Kumar[3]; *[1]Indian Institute of Technology Bombay, Mumbai, India; [2]Clarity Bio Systems*

India Pvt Ltd, Pune, India; [3]osmania medical college, Hyderabad, India

TP 079 **Very large-scale cerebrospinal fluid proteomics for biomarker discovery in multiple sclerosis**; Jakob Bader[1]; Christine Makarov[2]; Sabrina Richter[3]; Friederike Held[2]; Patricia Skowronek[4]; Maximilian Strauss[5]; Constantin Ammar[4]; Marvin Thielert[4]; Wen-Feng Zeng[4]; Isabell Bludau[4]; Benjamin Schubert[3]; Fabian Theis[3]; Christiane Gasperi[2]; Bernhard Hemmer[2]; Matthias Mann[1]; *[1]Department of Proteomics, Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Clinical Neuroimmunology Unit, University Hospital rechts der Isar, Technical University Munich, Munich, Germany; [3]Institute of Computational Biology, Helmholtz center Munich, Neuherberg, Germany; [4]Department of Proteomics, Max Planck Institute of Biochemistry, Martinsried, Munich, Germany; [5]NNF 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 Tan[3]; Samantha J Emery-Corbin[1, 2]; Jumana M Yousef[1, 2]; Ahmed Mohamed[2, 4]; Andrew Evans[5]; Seong-Seng Tan[6]; Shen-Yang Lim[3]; Han-Joon Kim[7]; Andrew I Webb[1, 2]; *[1]Advanced Technology and Biology Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Australia; [2]Department of Medical Biology, University of Melbourne, Parkville, Australia; [3]Faculty of Medicine, University of Malaya, Kuala Lumpur, Malaysia; [4]Bioinformatics Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Australia; [5]Movement Disorders Service, Department of Neurology, Royal Melbourne Hospital, Parkville, Australia; [6]Department of Medicine, Royal Melbourne Hospital, Parkville, Australia; [7]Department 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 Nasuhidehnavi[1]; Mahbobeh Lesani[2]; Jarrod A Roach[1]; Monica Ness[1]; Micah D'Armand De Chateauviex[1]; Laura-Isobel McCall[1, 2]; *[1]University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; [2]University 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 Charkoftaki[1]; Reza Aalizadeh[2]; Alvaro Santos-Neto[3]; Wan Ying Tan[4]; Emily A. Davidson[4]; Varvara Nikolopoulou[2]; Yewei Wang[4]; Brian Thompson[4]; Tristan Furnary[5]; Ying Chen[4]; Elsio Wunder[4]; Andreas Coppi[1]; Wade Schulz[1]; Akiko Iwasaki[1, 6]; Richard W. Pierce[1]; Charles S. Dela Cruz[1]; Gary V. Desir[1]; Naftali Kaminski[1]; Shelli Farhadian[1]; Kirill Veselkov[4, 7]; Rupak Datta[1]; Melissa Campbell[8]; Nikolaos S. Thomaidis[2]; Albert I. Ko[4]; David C. Thompson[4]; Vasilis Vasiliou[4]; *[1]Yale University, New Haven, CT; [2]National and Kapodistrian University of Athens, Athens, Greece; [3]University of São Paulo, São Carlos, Brazil; [4]Yale School of Public Health, New Haven, CT; [5]Harvard Medical School, Boston, MA; [6]Howard Hughes Medical Institute, Chevy Chase, MD; [7]Imperial College, London, London, United Kingdom; [8]Duke 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 Weise[1]; Sarah Samorodnitsky[3]; Carmen Martin-Alonso[4]; Erick Lock[3]; Subina Mehta[2]; Pratik D Jagtap[2]; Chris Wendt[1, 5]; Timothy J Griffin[2]; *[1]Department of Medicine, University of Minnesota, Minneapolis, MN; [2]Biochemistry, Mol. Biology and Biophysics, University of Minnesota, Minneapolis, MN; [3]Division of Statistics, School of Public Health, University of Minnesota, Minneapolis, MN; [4]Harvard-MIT Division of Health Sciences and Technology, MIT, Cambridge, Massachusetts; [5]Minneapolis 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 Vykoukal[1]; Taketo Kato[2]; Hiroyuki Katayama[1]; Allison Stewart[1]; Ehsan Irajizad[1]; Yining Cai[1]; Fuchung Hsiao[1]; Jennifer B Dennison[1]; Edwin J Ostrin[1]; Hai T Tran[1]; Carl M Gay[1]; Lauren A Byers[1]; Johannes Fahrmann[1]; Samir M Hanash[1]; *[1]The University of Texas MD Anderson Cancer Center, Houston, TX; [2]Nagoya University, Nagoya, Japan*

TP 085 **Proteomics identification of a potential biomarker of the malnutrition associated Konzo disease in human blood plasma samples**; Victor Fourcassié[1]; Matthew S. Bramble[2]; Florence Roux-Dalvai[1]; Neerja Vashist[3]; Dieudonné Mumba Ngoyi[4]; Desiré Tshala-Katumbay[4]; Éric Vilain[5]; Arnaud Droit[1, 6]; *[1]Proteomics platform, CHU de Québec - Université Laval Research Center, Quebec City, Québec; [2]Center for Genetic Medicine Research, Children's Research Institute, Children's National Hospital, Washington, DC USA, Washington, DC; [3]Center for Genetic Medicine Research, Children's Research Institute, Children's National Hospital, Washington, DC; [4]National Institute of Biomedical Research, Kinshasa, The Democratic Republic Of Congo; [5]Department of Genomics and Precision Medicine, The George Washington University School of Medicine and Health Sciences, Washington, DC; [6]Computational 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 Glass[1]; Todd A. Byers[2]; Darshpreet Kaur Saini[1]; Charles T. Bowen[1]; Bibhudutta Rout[1]; *[1]University of North Texas, Denton, TX; [2]University of North Texas, Denton, Texas*

TP 087 **Dual-column ZENO-TOF System to Achieve Robust and High-Quality Plasma Proteomics**; Yi (jimmy) Zeng[1]; Hao Qian[1]; Mark Marispini[1]; Jessica Chan[1]; Megan Mora[1]; Robert Zawada[1]; Philip Ma[1]; Bruce Wilcox[1]; *[1]PrognomiQ 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 Abid[1]; Haowen Qiu[2, 3]; Bridget A. Tripp[3]; Aline de Lima Leite[3]; Heidi E. Roth[1]; Jiri Adamec[4]; Robert Powers[1, 3, 5]; James W. Checco[1, 3]; *[1]Department of Chemistry, University of Nebraska-Lincoln, LINCOLN, NE; [2]Center for Biotechnology, University of Nebraska-Lincoln, LINCOLN, NE; [3]The Nebraska Center for Integrated Biomolecular Communication (NCIBC), University of Nebraska-Lincoln, LINCOLN, NE; [4]Department of Biochemistry, University of Nebraska-Lincoln, LINCOLN, NE; [5]Redox Biology Center, University of Nebraska-Lincoln, LINCOLN, NE*

TP 089 **2D LC-MS/MS with Direct Digestion to Enhance Quantitation of Monkey Serum hIDUA in the Presence of ADA and Endogenous Enzyme**; Wenchu Yang[1]; Drew Tietz[2]; Jiang Wu[2]; Sarah Yuan[2]; John Chen[1]; Chengjie Ji[1]; *[1]NovaBioAssays, Woburn, MA; [2]Sigilon 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 Pakkiri[1]; Lik Hang Wu[2]; Eugene Goh[2]; Poh Leong Lim[2]; A. Mark Richards[2, 3, 4]; Chester L. Drum[2, 3, 5]; *[1]National university of Singapore, Singapore, Singapore; [2]National University of Singapore, Singapore, Singapore; [3]cardiovascular research institute, Singapore, Singapore; [4]Christchurch heart institute, Univ. of Otago, Christchurch central city, New Zealand; [5]national university hospital, Singapore, Singapore*

TP 091 **A Universal Surrogate Matrix Assay for Urea Analysis in Biological Matrix to Support Clinical Pharmacokinetic Studies of Respiratory Diseases**; Yang

Tang[1]; Micheal Van Parys[2]; Xiaorong Liang[1]; Brian Dean[1]; Liuxi Chen[1]; [1]*Genentech Inc., South San Francisco, CA;* [2]*Labcorp, Madison, Wi*

TP 092 **A multiplexed mass spectrometric assay of 42 biomarkers for high-throughput screening obesity-related clinical samples**; Taitu Lin[1]; Panshak Dakup[1]; Athena A. Schepmoes[1]; Thomas L. Fillmore[1]; Adam C. Swensen[1]; Tong Zhang[1]; James P. Delany[2]; Bret H. Goodpaster[2]; Jie Pu[3]; Tujin Shi[1]; Jun Qu[3]; Wei-Jun Qian[1]; [1]*PNNL, Richland, WA;* [2]*AdventHealth, Orlando, FL;* [3]*University 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 Tu[1]; Vyncent Nguyen[2]; Km Shams Ud Doha[2]; Alex Abreu[1]; Sarah Baron[1]; Didar Asik[2]; Scott J. Jacobia[1]; Andrew M. Campbell[1]; [1]*Thermo Fisher Scientific, Grand Island, NY;* [2]*Thermo 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. Whelan[1]; Nathan Hendricks[1]; Zachary L. Dwight[1]; Qin Fu[2]; Annie Moradian[1]; Jennifer E. Van Eyk[2]; Susan M. Mockus[1]; [1]*Precision Biomarker Laboratories, Cedars-Sinai Medical Center, Beverly Hills, CA;* [2]*Smit 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 Ömer[1]; Markus Langsdorf[1]; Tuan Hai Pham[1]; Cornelia Röhring[1]; Therese Koal[1]; [1]*biocrates 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 Hsieh[1]; Mei-Lien Chen[2]; Pei-Wei Wang[2, 3]; Wen-Po Cheng[1]; Yu-Fang Huang*[2]; [1]*Department of Safety, Health and Environmental Engineering, National United University, Miaoli, Taiwan, Miaoli, Taiwan;* [2]*Institute of Environmental and Occupational Health Sciences, National Yang-Ming Chiao Tung University, Taipei, Taiwan;* [3]*Department 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 Dou[1]; Hiroyuki Katayama[2]; Ehsan Irajizad[2]; Yining Cai[2]; Johannes Fahrmann[2]; Jody Vykoukal[2]; Yihui Chen[2]; Ali Hussein Abdel Sater[2]; Edwin Ostrin[2]; Jaffer Ajani[2]; Samir Hanash[2]; [1]*MD Anderson Cancer Center, Houston, TX;* [2]*MD 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 Shen[1]; Jie Pu[1]; Chao Xue[1]; Wei-Jun Qian[2]; Cornelia L Boeser[3]; Claudia Martins[3]; Scott M Peterman[3]; Jun Qu[1, 4]; [1]*University at Buffalo, Buffalo, NY;* [2]*Pacific Northwest National Lab, richland, WA;* [3]*ThermoFisher Scientific, San Jose, CA;* [4]*New 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 Przybylski[1]; Pascal Wiegand[1]; Tamsila Khan[1]; Stefan Maeser[1]; Wolfgang Kleinekofort[1]; Andreas Hahn[2]; [1]*Centre for Analytical Biochemistry and Biomedical Mass Spectrometry, Rüsselsheim am Main, Germany;* [2]*Department 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 Shi[1]; Eric Kuhn[1]; Karen Yuan[1]; Yogesh Chutake[1]; Vaishali Dixit[1]; Michele Mayo[1]; Joyoti Dey[1]; Bin Yang[1]; Haojing Rong[1]; Phillip Liu[1]; Dirk M Walther[1]; Chris De Savi[1]; Kirti Sharma[1]; [1]*Kymera Therapeutics, Watertown, MA*

TP 102 **Serum N-Glycan Profiling of Patients with Narcolepsy type 1 Using LC-MS/MS** ; Akeem Adeyemi Sanni[1]; Md Abdul Hakim[1]; Mona Goli[1]; Samer El Hayek[2]; Farid Talih[3]; Bartolo Lanuzza[4]; Firas Kobeissy[5, 6]; Giuseppe Plazzi[7, 8]; Stefania Mondello[9]; Raffaele Ferri[4]; Yehia Mechref[1]; [1]*Texas Tech University, Lubbock, TX;* [2]*Department of Psychiatry and Behavioral Sciences, University of Miami Miller School of Medicine, Miami, FL;* [3]*Department of Psychiatry, Faculty of Medicine, American University of Beirut, Beirut, Lebanon;* [4]*Sleep Research Centre, Department of Neurology IC, Oasi Research Institute- IRCCS, Troina, Italy;* [5]*Faculty of Biochemistry and Molecular Genetics, American University of Beirut, Beirut, Lebanon, Beirut, Lebanon;* [6]*Morehouse School of Medicine (MSM), Center for Neurotrauma, Multiomics & Biomarkers, Department of Neurobiology, Atlanta, Georgia;* [7]*IRCCS, Istituto delle Scienze Neurologiche di Bologna, Bologna, Italy;* [8]*Department of Biomedical, Metabolic and Neural Sciences, University of Modena and Reggio Emilia, Modena, Italy;* [9]*Department 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 Weiner[1]; Mathias Sauer[1]; Nicholas Ashton[1]; Pedro Rosa-Neto[2]; Henrik Zetterberg[1, 3]; Kaj Blennow[1, 3]; Johan Gobom[1, 3]; [1]*University of Gothenburg, Gothenburg, Sweden;* [2]*McGill University, Montreal, Québec;* [3]*Sahlgrenska University Hospital, Gothenburg, Sweden*

TP 104 **Development of a Highly-specific LC-MS/MS based Quantitative Fecal Occult Blood Test for Canine**; Zhiyu Li[1]; Hefeng Zhang[1]; Siyu Liu[1]; Zhiren Yu[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; [1]*WuXi AppTec, Shanghai, China*

TP 105 **Evaluating co-expression of tagged proteins in isolated EVs with attomole sensitivity**; Michael A Shaw[1]; Dmitriy Verkhoturov[2]; Seonhwa Lee[3]; Stanislav Verkhoturov[2]; Michael J. Eller[1]; Alexander Revzin[3]; Emile A. Schweikert[2]; [1]*Department of Chemistry and Biochemistry, California State University Northridge, Northridge, California;* [2]*Department of Chemistry, Texas A&M University, College Station, Texas;* [3]*Department 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 Kandi[1]; Qin C Ji[2]; John P. Savaryn[2]; Sarah Blink Polakow[2]; Gary J Jenkins[2]; Kenneth Ruterbories[2]; Mary Saltarelli[2]; Mario Richter[2]; [1]*Abbvie, North Chicago, IL;* [2]*AbbVie, 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 Wang[1]; Nan Jiang[2]; Linzhen Song[2]; Huanjun Ling[2]; Junli Gao[2]; Junshun Gao[2]; Shenpeng Ying[3]; Qi Chen[3]; [1]*Hangzhou Cosmos Wisdom Mass Spectrometry Center of Zhejiang University Medical School, Hangzhou, China;* [2]*Hangzhou Cosmos Wisdom Mass Spectrometry Center of Zhejiang University Medical School, Hangzhou, China;* [3]*Taizhou Central Hospital, Taizhou, China*

TP 108 **Investigation of systemic inflammation induced FcRn dysregulation with sensitive LC-FAIMS-dCV-MRM**; Chao Xue[1]; Qingqing Shen[1]; Jie Pu[1]; Yang Liu[1]; Ming Zhang[1]; Jun Qu[1, 2]; [1]*University at Buffalo, Buffalo, NY;* [2]*New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY*

TP 109 **LC-MS based Discovery of Plasma Phosphopeptide Markers for Alzheimer's Disease Staging and Clinical trials**; Kyungdo Kim[1]; Min-Kyung Jun[1]; Se Hwan Jang[1]; Byeong C. Kim[2]; Zee-yong Park[1]; *[1]School of Life Science, Gwangju Institute of Science and Technology, Cheomdangwagiro123, Buk-gu, Gwangju, South Korea; [2]Department of Neurology, Chonnam National University Hospital, Gwangju, South Korea*

TP 110 **NanoLC-timsTOF platform-assisted analysis of glycated 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 Huang[3]; Eric F Zaniewski[1, 2]; Soroush Hajizadeh[1, 2, 4]; Benedikt C, Clemens[1, 2]; David Bergen[3]; Jesse D. Canterbury[5]; Michael W. Senko[3]; Graeme C McAlister[3]; 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 Qiu[3]; Vladimir Ignatchenko[2]; Danny Vesprini[4]; O. John Semmes[5]; Julius O Nyalwidhe[5]; Stanley Liu[1, 4]; Paul C Boutros[3]; 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, 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 Higginson[1]; Jasmin Werner[1]; Stefania Maneta-Stavrakaki[1]; Lauren Ford[1]; Dani Simon[1]; Yuchen Xiang[1]; Jagtar Dhanda[2]; Zoltan Takats[1]; *[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. Wang[1]; Stephen Kurzyniec[1]; Erin Strom[2]; Tammy Jones-Lepp[2]; Amanda Leisgang[2]; Andrew Ortiz[2]; Jefferson Kinney[2]; Yoshiyuki Okamura[1]; *[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 Perciaccante[1]; Kate Brown[1]; Tapan K Maity[1]; Massimiliano Bissa[2]; Genoveffa Franchini[2]; Daniel H Appella[3]; Ettore Appella[1]; Lisa M Jenkins[1]; *[1]Laboratory of Cell Biology, Center for Cancer Research, National Cancer Institute, Bethesda, MD; [2]Vaccine Branch, Center for Cancer Research, National Cancer Institute, Bethesda, MD; [3]Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD*

TP 116 **Millions of cellular drug assays created by dose-resolved (phospho)proteomics reveal drug mechanism of action and decrypt post-translational modifications**; Jana Zecha[1]; Florian P. Bayer[1]; Nicola Berner[1]; Stephan Eckert[1]; Svenja Wiechmann[1]; Matthew The[1]; Julian Mueller[1]; Karl Kramer[1]; Guillaume Medard[1]; Mathias Wilhelm[1]; Annika Schneider[1]; Maria Reinecke[1]; Julia Woortman[1]; Severin Lechner[1]; Patroklos Samaras[1]; Ludwig Lautenbacher[1]; Firas Hamood[1]; Polina Prokofeva[1]; Stephanie Heinzlmeier[1]; Benjamin Ruprecht[1]; Bernhard Kuster[1]; *[1]Technical University of Munich, Freising, Germany*

TP 117 **HDAC inhibitors induce proteome remodeling of diverse lung cancer cells**; Chuwei Lin[1]; Devin Schweppe[1]; *[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 Jain[1]; Rafaela Muniz De Queniroz[2]; Jayanta K. Chakrabarty[1]; Lipi Das[1]; Carol Prives[2]; Lewis M. Brown[1]; *[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 Lempiainen[1]; Yixuan (axe) Xie[1]; Angela C Hirbe[2]; Benjamin A Garcia[1]; *[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 Adachi[1]; Hirokazu Shoji[2]; Masahiko Aoki[2, 3]; Hidekazu Hirano[2]; Yuichi Abe[1]; Kazufumi Honda[4]; Takeshi Tomonaga[1]; Kenji Mizuguchi[1]; Takaki Yoshikawa[2]; Narikazu Boku[5]; *[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 Ahuja[1]; Becki Dudley[2]; Abby J. Chiang[3]; Matthew S. Glover[3]; Lisa H Cazares[3]; Luca Melchiori[2]; Robert Wilkinson[2]; Dmitry Gabrilovich[3]; Des Jones[2]; Sonja Hess[3]; *[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 Burton[1]; Deng Pan[2]; Joanna Bons[1]; Rosemary Bai[2]; Chira Chen-Tanyolac[2]; Deborah Collyar[2]; Christie L Hunter[3]; Philippe Gascard[2]; Thea D Tlsty[2]; Birgit Schilling[1]; *[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 Hassan[1]; Danthasinghe Waduge Badrajee Piyarathna[2]; Vasanta Putluri[2]; Roni J. Bollag[3]; Martha K Terris[3]; Leomar Y Ballester[4]; Yair Lotan[5]; Cristian Coarfa[2]; Nagireddy Putluri[2]; *[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 inHCT 116 Colon Cancer Spheroids During Growth**; Catherine B Edgington[1]; Nicole C. Beller[2]; Amanda B. Hummon[2]; *[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 Buhman[1]; Dorothy Teegarden[1]; *[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 Xiao[1]; Yi Liu[1]; Zongtao Lin[2]; Jing Pei[3]; Guangrong Zheng[1]; Dongwen Lv[3, 4]; *[1]Department of*

Medicinal Chemistry, College of Pharmacy, University of Florida, Gainesville, FL; [2]Department of Biochemistry and Molecular Biophysics, Washington University in St. Louis, St Louis, MO; [3]Department 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; [4]Mays 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 Liu[1]; Yixuan (axe) Xie[1]; Zongtao Lin[1]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

TP 128 **SUMO inhibition unveils the dark immunopeptidome in acute myeloid leukemia**; Léa Christophe[1]; Mirela Pascariu[1]; Chantal Durette[1]; Eric Bonneil[1]; Joel Lanoix[1]; Marie-Pierre Hardy[1]; Krystel Vincent[1]; Claude Perreault[1, 2]; Pierre Thibault[1, 3]; *[1]Institute of Research in Immunology and Cancer, Université de Montréal, Montreal, QC; [2]Department of Medicine, Université de Montréal, Montréal, Québec; [3]Department of Chemistry, Université de Montréal, Montréal, Québec*

TP 129 **Metabolic Pathways of Monounsaturated Lipids Revealed by In-depth Structural Lipidomics by Mass Spectrometry**; Simin Cheng[1]; Zheng Ouyang[1]; Xiaoxiao Ma[1]; *[1]Tsinghua University, Beijing, China*

TP 130 **Investigating Lipid Sources Contributing to Resistance to Lysosomal Autophagy Inhibition in Melanoma**; Sandra L. Harper[1]; Vaibhav Jain[2]; Ravi K. Amaravadi[2]; David W. Speicher[1]; Aaron R. Goldman[1]; *[1]The Wistar Institute, Philadelphia, PA; [2]University of Pennsylvania, Philadelphia, PA*

TP 131 **Cell Viability, Purity, and Drug-Protein Interactions of Novel Gold (I) Compounds Within Various Cancer Types**; Kyle L. Wilhelm[1]; Charli Worth[1]; Neda Fezi[1]; Shyam Pokhrel[2]; Ahmad Ahmad[2]; Mitchell Bruce[2]; Alice Bruce[2]; Joseph Taube[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX; [2]University of Maine, Orono, ME*

TP 132 **Verification of Serum Biomarkers for High-Grade Serous Ovarian Carcinoma Recurrence by Targeted Proteomics**; Deborah Wenk[1]; Shahbaz Khan[1]; Vladimir Ignatchenko[1]; Marcus Q. Bernardini[2, 3]; Thomas Kislinger[1, 4]; *[1]Princess Margaret Cancer Centre, University Health Network, Toronto, ON; [2]Division of Gynecologic Oncology, Princess Margaret Cancer Centre, University Health Network, Toronto, ON; [3]Department of Obstetrics and Gynaecology, University of Toronto, Toronto, ON; [4]Department 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 Ma[1]; Soojin Park[2]; Thu-Huyen Pham[2]; Andro Botros[2]; Sylvia R. Yun[2]; Eun Young Park[2]; Olga Kim[2]; Grace Grimsley[3]; Jaeyeon Kim[2]; Richard R. Drake[3]; Facundo M. Fernandez[1]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; [2]Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, IN; [3]Department 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. Holt[1]; Yongchao Dou[1]; Meggie N. Young[1]; Antrix Jain[1]; Alexander B. Saltzman[1]; Jonathan T. Lei[1]; Kyle D. Drinnon[1]; Sung Han Kim[1]; Meenakshi Anurag[1]; Bing Zhang[1]; Anna Malovannaya[1]; Seth P Lerner[1]; *[1]Baylor College of Medicine, Houston, Texas*

TP 135 **Identifications of metabolic changes upon microbiome depletion in pancreatic tumor bearing mice models**; Dominik Awad[1]; Li Zhang[1]; Xiaoyi Li[1]; Peter Sajjakulnukit[1]; Anthony Andren[1]; Costas Lyssiotis[1]; *[1]University 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 Shaheed[1]; Fenna E.M. Van De Leemkolk[2]; Corinna M Snashall[1]; Maria Letizia Lo Faro[1]; Chris W. Sutton[3]; Jan H.N. Lindeman[2]; Rutger J. Ploeg[1, 2]; *[1]Nuffield Department of Surgical Sciences, University of Oxford, Oxford, United Kingdom; [2]Department of Surgery, Transplant Center Leiden University Medical Center, Netherlands; [3]Institute 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 Keating[1]; Charles A. Wolfe[2]; Andréia de Melo Porcari[2]; Alexander Makarov[3]; Livia S. Eberlin[2]; *[1]University of Texas at Austin, Austin, TX; [2]Division of Surgical Oncology, Baylor College of Medicine, Houston, Texas; [3]Thermo 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. Wyche[1]; Corinne Thomas[1]; Melanie Anderson[2]; Brad R. Evans[2]; Kevin P. Bateman[2]; Theodore R. Sana[1]; *[1]Merck & Co., Inc., Cambridge, MA; [2]Merck & 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 Chai[1]; Hou-Chun Huang[1]; Yu-Hsuan Chen[1]; Jia-Fang Tsai[2]; Yi-Hua Liao[2, 3]; Cheng-Chih Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei City, Taiwan; [2]Department of Dermatology, National Taiwan University Hospital, Taipei City, Taiwan; [3]Department 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. Qasrawi[1]; Rania M Khan[1]; Evgeniy V. Petrotchenko[1]; Manuel Montero-Odasso[2]; Christoph H. Borchers[1, 3, 4, 5]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [2]St. Joseph's Health Care, University of Western Ontario, London, ON; [3]Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [4]Division of Experimental Medicine, McGill University, Montreal, QC; [5]Department 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 Guo[1]; Courtney Patterson[2]; Richard Gibson[2]; Kristine Van Natta[2]; Stephanie N. Samra[2]; *[1]Thermo Fisher Scientific, Roseville, MN; [2]Thermo 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 Venkatesh[1]; Alex Yuile[2]; Matthew J McKay[1]; Sathya Narayanan[2]; Helen Wheeler[2]; Malinda Itchins[2]; Nick Pavlakis[2]; Stephen J Clarke[2]; Mark P Molloy[1]; *[1]School of Medical Sciences, The University of Sydney, Sydney, Australia; [2]Department 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 Goda[1]; Tsuyoshi Nakanishi[2]; Junichi Masuda[1]; Natsuka Kimura[3]; Kenichi Aizawa[3]; *[1]SHIMADZU Corporation, Kawasaki, Japan; [2]SHIMADZU Corporation, Kyoto, Japan; [3]Jichi Medical University, Shimotsuke, Japan*

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 Hrabák[4]; Lukáš Fojtík[1, 2]; Petr Novák[1, 2]; *[1]Department of Biochemistry, Charles University, Prague, Czech Republic; [2]Institute of Microbiology of the CAS, v. v. i., Prague, Czech Republic; [3]Institute of Biotechnology of the CAS, v. v. i., Prague, Czech Republic; [4]Biomedical 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 Petritis[1]; Samantha L Isenberg[1]; C. Austin Pickens[1]; Carla Cuthbert[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

TP 146 **Facile and expediated high-throughput sample preparation prior to analysis of clinically relevant free hormones from serum**; M James Ross[1]; Gabriel Odugbesi[1]; *[1]MilliporeSigma, 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 Mignet[1]; Alexandre Kulus[2]; Matthieu Allez[5]; Yannis Nicolas Francois[2]; Rabah Gahoual[1]; *[1]Unité de Technologies Chimiques et Biologiques pour la Santé, UMR8258 CNRS, Inserm U1022, Faculty of Pharmacy, Université Paris Cité, Paris, France; [2]Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, Strasbourg, France; [3]Unité de Technologies Chimiques et Biologiques pour la Santé (UTCBS), CNRS UMR8258, Inserm U1022, Université de Paris, France; [4]Laboratoire de Toxicologie Biologique, Hôpital Lariboisière, Assistance Publique – Hôpitaux de Paris (AP-HP), France; [5]Hopital Saint-Louis, Assistance Publique – Hôpitaux de Paris (AP-HP), Paris, France*

TP 148 **Simultaneous Quantification of 13 Clinically Significant Simple and Macrocyclic Trichothecenes in Human Urine Using Liquid Chromatography with Tandem Mass Spectrometry**; Claudia C Beck[1]; Matthew R McIntyre[1]; Dennis G Hooper[1]; *[1]Realtime 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 Kumar[1]; Coreen L. Johnson[2]; Michael Keating[1]; James J. Dunn[2]; Min Woo Sun[3]; Robert Tibshirani[4]; Rachel D. Downey[5]; Lindsey M. Kirkpatrick[6]; Livia S. Eberlin[1]; *[1]Baylor College of Medicine, Department of Surgery, Houston, Texas; [2]Texas Children's Hospital, Dept. of Pathology, Houston, Texas; [3]Stanford University, Departments of Biomedical Data Sciences and Statistics, Stanford, CA, Texas; [4]Stanford University, Departments of Biomedical Data Sciences and Statistics, Stanford, CA; [5]Dell Children's Medical Center, Austin, TX; [6]Riley Hospital for Children, Dept. of Pediatric Infectious Diseases, Indianapolis, IN*

TP 150 **Therapeutic Drug Monitoring Using Miniature Mass spectrometer for ICU**; Jiexun Bu[1]; Nan Zhang[1]; Wenpeng Zhang[2]; Zheng Ouyang[2]; *[1]PURSPEC Technology (Beijing) Ltd., Beijing, China; [2]Department 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 Tan[1]; Troy Puar[1]; Daryl Hee[1]; *[1]CHANGI GENERAL HOSPITAL, Singapore, Singapore*

TP 152 **A complete, automated end-to-end workflow for high-throughput therapeutic drug monitoring using Evosep MRM**; Angela Mc Ardle[1]; Magnus Huusfeldt[2]; Bharath Kumar Raghuraman[1, 3]; Dorte Bekker-Jensen[1]; Ole Vorm[1]; Nicolai Bache[1]; *[1]Evosep, Odense, Denmark; [2]Evosep, Odense, Denmark; [3]Department 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 MacNamara[1]; Samantha L Isenberg[1]; Carla Cuthbert[1]; Konstantinos Petritis[1]; *[1]CDC, 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-Williams[1]; Ruiting Li[2]; Amanda Bwint[3]; Bo Wen[2]; Duxin Sun[2]; Marc Scheetz[4]; Kevin J. Downes[3]; Athena F Zuppa[3]; Manjunath P. Pai[2]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Michigan Ann-Arbor, Ann Arbor, MI; [3]Children's hospital of Philadelphia, Philadelphia, Pennsylvania; [4]Midwestern 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 Jiang[1]; Janusz B Pawliszyn[1]; *[1]University 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 Ardle[1]; Ole Vorm[1]; Nicolai Bache[1]; Martin Overgaard[2]; Christian Ravnsborg[1]; *[1]Evosep Biosystems, Odense, Denmark; [2]Odense 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 Espourteille[1]; Terry Bates[2]; *[1]Bruker Corporation, Billerica, MA; [2]Bruker 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 Lai[2]; Kun-Chen Lee[2, 4]; Te-I Weng[1, 2, 5]; *[1]Department and Graduate Institute of Forensic Medicine, College of Medicine, National Taiwan University, Taipei, Taiwan; [2]Forensic and Clinical Toxicology Center, National Taiwan University Hospital, Taipei, Taiwan; [3]Department of Pharmacy, College of Medicine, National Taiwan University, Taipei, Taiwan; [4]Department of Laboratory Medicine, National Taiwan University Hospital, Taipei, Taiwan; [5]Department 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 Hadisurya[1]; Zhuojun Luo[1]; Xiaofeng Wu[2]; Anton B. Iliuk[3]; Ronald S Boris[4]; W. Andy Tao[1, 3, 5]; *[1]Department of Biochemistry, Purdue University, West Lafayette, Indiana; [2]Department of Chemistry, Purdue University, West Lafayette, Indiana; [3]Tymora Analytical Operations, West Lafayette, Indiana; [4]Department of Urology, Indiana University School of Medicine, Indianapolis, Indiana; [5]Department 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 Johnson[1]; Nicholas Chestara[2]; Yoshiyuki Okamura[3]; *[1]Shimadzu Scientific Instruments, Carlsbad, CA; [2]DPX Technologies, La Jolla, CA; [3]Shimadzu Scientific Instrument, Columbia, Maryland*

TP 161 **Rapid diagnosis of brain tumors by onco-metabolic detection using miniature mass spectrometry system**; Junhan Wu[1]; Xinqi Fang[2]; Haoyue Zhang[1]; Bin Jiao[1]; Nan Wang[3]; Jiexun Bu[3]; Xiao Chen[1]; Wei Hua[2]; Ying Mao[2]; Wenpeng Zhang[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China; [2]Huashan Hospital, Fudan University, Shanghai, China; [3]PURSPEC Technology (Beijing) Ltd., Beijing, China*

TP 162 **Human Biofluid Benchmark Study comparing different workflows for deep and unbiased Clinical Proteomics**;

Carleen M Kluger[1]; Giada Marino[1]; Nagarjuna Nagaraj[1]; Samira Vautrin[1]; Till Kindel[1]; Elena Kunold[1]; Stefanie Tebbe[1]; Frank Rolfs[1]; Doris Staudt[1]; Olga Shatnyeva[2]; Andreas Tebbe[1]; *[1]Evotec München GmbH, Neuried, Germany; [2]Evotec 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 Gao[1]; Xuefei Zhong[1]; Yuan Mao[1]; Ning Li[1]; Albert Torri[2]; *[1]Analytical Chemistry Group, Regeneron Pharmaceuticals Inc., Tarrytown, New York; [2]Bioanalytical Sciences, Regeneron Pharmaceuticals Inc., Tarrytown, New York*

TP 164 **Following molecular changes during wound skin healing with topical statin treatment**; Lilian Valadares Tose[1]; Ahmed Hawash[2]; Ivan Jozic[2]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]University of Miami, Miami, FL*

TP 165 **CardioCarePack – personalized medicine system to improve live quality of patients suffering from cardiac arrhythmias**; Maciej Stopa[1]; Rafał Szewczyk[1, 2]; Anna Lenartowicz[2]; Julia Mironenka[2]; Katarzyna Krupczyńska - Krupczyńska - Stopa[1, 2]; Adrian Soboń[1, 2]; Leszek Kalinowski[3]; Adrianna Radulska[3]; Tomasz Borkowski[3]; Ewelina Marciniak[3]; *[1]Bioanalytic Sp. z o.o., Gdansk, Poland; [2]LabExperts sp. z o. o., Gdańsk, Poland; [3]Gdansk 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 Rajapakshe[2]; Emily Garnett[1, 2]; Sridevi Devaraj[1, 2]; *[1]Department of Pathology and Immunology, Baylor College of Medicine, One Baylor Plaza, Houston, TEXAS; [2]Department 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 Lin[1]; Austin B. Moyle[1, 2]; Victor A. Beaumont[3]; Lucy L. Liu[4]; Sharon Polleck[4]; Don L. Rempel[1]; Haijun Liu[1]; Heliang Shi[5]; Jason C. Rouse[4]; Hai-Young Kim[4]; Ying Zhang[4, 6]; Michael L. Gross[1]; *[1]Washington university in St louis, St Louis, MO; [2]AbbVie Inc., North Chicago, IL; [3]Pfizer, Inc., Sandwich, United Kingdom; [4]Pfizer, Inc., Andover, MA; [5]Pfizer, Inc., New York City, NY; [6]Sarepta Therapeutics, Inc., Cambridge, MA*

TP 168 **Mono- and Intralink Filter (Mi-Filter) To Reduce False Identifications in Cross-Linking Mass Spectrometry Data**; Xingyu Chen[1]; Carolin Sailor[1]; Kai Michael Kammer[1]; Julius Fürsch[1]; Eri Sakata[2]; Markus rainer Eisele[2]; Riccardo Pellarin[3]; Florian Stengel[1]; *[1]University of Konstanz, Konstanz, Germany; [2]University Medical Center Göttingen, Göttingen, Germany; [3]Institut Pasteur, Paris, France*

TP 169 **Chemoproteomic approaches to decipher novel mechanisms of non-vesicular cholesterol transport**; Miranda Villanueva[1]; Nikolas Burton[2]; Andrew Palmer[2]; Sho Takechi[2]; Rohith Nagari[2]; Liujuan Cui[2]; Peter Tontonoz[2]; Keriann Backus[2]; *[1]UCLA, LOS ANGELES, CA; [2]UCLA, Los Angeles, CA*

TP 170 **Investigating daptomycin–membrane interactions using mass spectrometry**; Tapasyatanu Dash[1]; Deseree Reid[1]; Michael T Marty[1]; *[1]The University of Arizona, Tucson, Arizona*

TP 171 **New regions of interaction revealed for Aquaporin-0 binding partners via XL-MS**; Carla O'Neale[1]; Zhen Wang[1]; Kevin Schey[1]; *[1]Vanderbilt University, Nashville, TN*

TP 172 **A photo-tagging approach for studying the interactions between model peptides and membrane lipids**; Jing Zhao[1]; Lipeng Qiao[1]; Yu Xia[1]; *[1]Tsinghua University, Beijing, China*

TP 173 **In vitro to In vivo Characterization of Amyloid Beta 1-42 using Mass Spectrometry-based Footprinting**; Cynthia (xinyi) Kuang[1]; Yanchun Lin[1]; Zhao Sun[2]; Andrew Yoo[2]; Michael L. Gross[3]; *[1]Washington University in St. Louis, St. Louis, MO; [2]Washington University School of Medicine, St. Louis, MO; [3]Washington university in St louis, St Louis, MO*

TP 174 **Ving: A New Tool in the Trans-Proteomic Pipeline for XL-MS Using Cleavable Cross-Linking Reagents**; Michael R. Hoopmann[1]; David D. Shteynberg[1]; Luis Mendoza[1]; Kamal Mandal[2]; Arun P. Wiita[2]; Eric W. Deutsch[1]; Robert L. Moritz[1]; *[1]Institute for Systems Biology, Seattle, WA; [2]University of California San Francisco, San Francisco, CA*

TP 175 **A Covalent Labeling-Mass Spectrometry Method for Identifying Protein Amyloid Inhibitors**; Kanitin Khamnong[1]; Richard W. Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

TP 176 **Optimized XL-MS workflows for membrane protein analysis**; Yi He[1]; Gregory J Dodge[2]; Barbara Imperiali[2]; Rosa Viner[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Massachusetts Institute of Technology, Cambridge, MA*

TP 177 **Carbene Crosslinking in Gas-Phase Peptide Ion Scaffolds**; Hongyi Zhu[1]; Václav Zima[1]; Emily Ding[1]; František Tureček[1]; *[1]University of Washington, Seattle, WA*

TP 178 **Dimethylthiourea as a Quencher in Hydroxyl Radical Protein Footprinting Experiments**; Anter A Shami[1]; Sandeep K. Misra[1]; Lisa Jones[2]; Joshua S. Sharp[1]; *[1]The University of Mississippi, University, MS; [2]University 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. Minkoff[1]; Heather L. Burch[1]; Jamison D. Wolfer[1]; Michael R. Sussman[1]; *[1]University of Wisconsin, Madison, WI*

TP 180 **Developing peptide-centric cleavable proximity labeling proteomics to study mitochondrial membrane protein topology**; Haorong Li[1]; Jiawei Ni[1]; Ryan Houston[2]; Shiori Sekine[2]; Ling Hao[1]; *[1]George Washington University, Washington, DC, DC; [2]University of Pittsburgh, Pittsburgh, PA*

TP 181 **Conventional cell fixation improves performance of in situ crosslinking mass spectrometry while preserving ultrastructure**; Andrew RM Michael[1]; Bruno C Amaral[1]; David C Schriemer[1]; *[1]University of Calgary, Calgary, AB*

TP 182 **Confidently Identifying protein-protein interactions by harmonizing cross-link scores with machine learning**; Pin-Lian Jiang[1]; Max Ruwolt[1]; Boris Bogdanow[1]; Fan Liu[1]; *[1]Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany*

TP 183 **Real-time library search improves the sensitivity and throughput of cross-link identification**; Max Ruwolt[1]; Yi He[2]; Diogo Borges[1]; William Barshop[2]; Rosa Viner[2]; Fan Liu[1]; *[1]Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; [2]Thermo Fisher Scientific, San Jose, CA*

TP 184 **High-throughput XL-MS analysis on a new high-resolution accurate mass platform**; Yi He[1]; Tabiwang Arrey[2]; Martin Zeller[2]; Nicolaie Eugen Damoc[2]; Rosa Viner[1]; *[1]ThermoFisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

TP 185 **Protein Footprinting Using Water Photolysis**; Oluwatosin A. Ogundairo[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

TP 186 **Development of Fast Photochemical Footprinting of Glycans for Topographical Analysis of Glycans**; Sandeep K. Misra[1]; Hao Liu[1]; Sidney Stuckett[1]; Joshua S. Sharp[1]; *[1]University of Mississippi, University, MS*

TP 187 **Cross-link assisted spatial proteomics to map sub-organelle proteomes and membrane protein topology**; Ying Zhu[1]; Kerem Can Akkaya[1, 2]; Diogo Borges Lima[1]; Max Ruwolt[1]; Cong Wang[1]; Martin Lehmann[2]; Fan Liu[1, 3]; *[1]Department of Structural Biology, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP),* *Berlin, Germany; [2]Core Facility Cellular Imaging, Leibniz Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; [3]Charité – Universitätsmedizin Berlin, Berlin, Germany*

TP 188 **Fluidic platform for enrichment of protein complexes for crosslinking-MS on a magnetic particle-based trap**; Shaunak Raval[1]; David C Schriemer[1]; Vladimir Sarpe[1]; Alex D Crowder[1]; Pauline Douglas[1]; Susan P Lees-Miller[1]; Danny Laurent[1]; *[1]University 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. Stahl[1]; Zachary J. Kirsch[2]; Trisha W. Brady[2]; Andrew J. Shultz[1]; Jennifer N. Rauch[1, 3]; Richard W. Vachet[1, 2]; *[1]Molecular & Cellular Biology Program, University of Massachusetts Amherst, Amherst, MA; [2]Department of Chemistry, University of Massachusetts Amherst, Amherst, MA; [3]Department of Biochemistry & Molecular Biology, University of Massachusetts Amherst, Amherst, MA*

TP 190 **Are these crosslinking results significant? Bring on the bootstrap!**; Lindsey D Ulmer[1]; Christopher N Woods[2]; Natalie L Stone[2]; Rachel E Klevit[2]; Matthew F Bush[1]; *[1]Department of Chemistry, University of Washington, Seattle, WA; [2]Department of Biochemistry, University of Washington, Seattle, WA*

TP 191 **Thrombin-DNA Aptamer Binding Investigated by DEPC Covalent Labeling-MS**; Zachary J Kirsch[1]; Jonathan Ashby[2]; Richard W. Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA; [2]Mount Holyoke College, Holyoke, MA*

TP 192 **Unique Protein Identifications Improve Protein-Protein Interaction Identification Rate in CRIMP 2.0**; D Alex Crowder[1]; Vladimir Sarpe[1]; David C Schriemer[1]; *[1]University 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 Vadi[1]; Alessio Corrado[1]; *[1]GSK vaccines, Siena, Italy*

TP 194 **Accelerating Drug Discovery using an Automated High-Throughput Desorption Electrospray Ionization Mass Spectrometry Platform**; Nicolas M. Morato[1]; Kai-Hung Huang[1]; Samadhi C. Kulathunga[1]; Veronica Feng[1]; Beinan Yang[1]; Jiang Yang[1]; Eric T. Dziekonski[1]; Timothy L. Ratliff[1]; Andrew D. Mesecar[1]; R. Graham Cooks[1]; *[1]Purdue 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 Meng[1]; Laixin Wang[1]; Yuhuan Ji[1]; Zhong Hong[1]; Aihua Liu[2]; *[1]Chongqing Denali Medpharma, Beibei District, China; [2]Alliance Pharma, Malvern, PA*

TP 196 **Quantitative Workflow for xC/UV/MS Data using a Single Vendor-Neutral Interface**; Anne Marie Smith[1]; Yury Zhukov[1]; Sofya Chudova[1]; Vitaly Lashin[1]; *[1]ACD/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 Xu[1]; Yongying Jiang[1]; Emilia Di Francesco[1]; Philip Jones[1]; *[1]Institute 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 Zhang[1]; Eric L Dane[2]; Jianing Wang[1]; *[1]Millennium Pharmaceuticals, Inc., cambridge, MA; [2]Koch 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 Xin[1]; Shuo Liu[2]; Karl Barry Sharpless[3]; Jiajia Dong[2]; Wenqing Shui[1]; *[1]ShanghaiTech University, Shanghai, China; [2]Shanghai Jiao Tong University, Shanghai, China; [3]The 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 Yang[1]; Md. Amin Hossain[1]; Christopher Singleton[1]; Brandon C. Miller[1]; Yifan Liu[1]; Roman Manestch[1]; Jeffrey N. Agar[1]; *[1]Northeastern 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. Wildburger[1]; Cristina Di Poto[1]; Jana Zecha[1]; Mahder Abate[1, 2]; Silke Reischl[3]; Erik Allman[1]; Lisa H. Cazares[1]; Bilican Bilada[3]; Sonja Hess[1]; *[1]AstraZeneca R&D, Gaithersburg, Maryland; [2]University of Maryland College Park, College Park, MD; [3]AstraZeneca, Molndal, Sweden*

TP 202 **Feasibility of nMS for large scale hit validation and screening through high compression**; Wenyi Hua[1]; Xidong Feng[1]; *[1]Pfizer Inc., Groton, CT*

TP 203 **Mass Spectrometry-based Barcoding and Screening Platform Designed for Quantitative Macromolecular Drug Delivery**; Ning Wang[1]; Nicole A. McNeer[1]; Alex Kentsis[1, 2]; *[1]Memorial Sloan Kettering Cancer Center, New York, New York; [2]Weill 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 Lv[1]; Tie Gao[1]; Hexing Song[1]; Luo Ji[1]; Hongxu Chen[1]; Lihai Guo[1]; *[1]SCIEX, China, Beijing, China*

TP 205 **Characterization of proteins in influenza virus vaccines by LC-MS/MS and CGE**; Xiaoxia Zhang[1]; Yang Song[1]; Ji Luo[1]; Hongxu Chen[2]; *[1]SCIEX, China, Shanghai, China; [2]SCIEX, China, Beijing, China*

TP 206 **Deep proteomic screening and validation for systematic discovery of molecular glue compounds and novel degrader targets**; Uli Ohmayer[1]; Martin Steger[2]; Bjoern Schwalb[2]; Anastasia Bednarz[2]; Sophie Machata[2]; Jutta Fritz[2]; Henrik Daub[2]; *[1]NEOsphere Biotechnologies GmbH, Planegg, Germany; [2]NEOsphere Biotechnologies GmbH, Planegg, Germany*

TP 207 **DRAFT: A Dose-Response Activity Finder Tool for drug target deconvolution in chemical proteomics experiments**; Praveen Kumar[1]; Heng Zhao[1]; Aarti Kawatkar[1]; Steven Novick[1]; *[1]AstraZeneca, Waltham, MA*

TP 208 **Strategy for Bioanalysis of Liposomal Drugs in Support of Bioequivalence Study**; Yuhuan Ji[1]; Jinzhi Liu[1]; Min Meng[1]; Xueyuan Zhang[2]; Chunlei Li[2]; Laixin Wang[1]; *[1]Chongqing Denali Medpharma Co.,Ltd, Chongqing, China; [2]CSPC Pharmaceutical Group Ltd, Shijiazhuang, China*

TP 209 **RokaiXplorer: An online tool for interactive analysis of proteomics and phospho-proteomics data**; Serhan Yilmaz[1]; Filipa Blasco Tavares Pereira Lopes[1]; Marzieh Ayati[2]; Mark Chance[1]; Mehmet Koyuturk[1]; *[1]Case Western Reserve University, Cleveland, OH; [2]The 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 Sun[1]; Hongxing Liu[1]; Jinyan Guo[1]; Ran Xiao[1]; Lei Wang[1]; *[1]Hebei 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 Sharma[1]; Reda Assal[1]; Shahid Rehan[1]; Katharina Duerr[1]; Laia Malet Sanz[1]; Adam Sanderson[1]; Jonathan Hopper[1]; Steven Charlton[1]; Ali Jazayeri[1]; Idlir Liko[1]; *[1]OMass Therapeutics, Oxford, United Kingdom*

TP 212 **Unbiased validation of degrader drug neosubstrates by high-sensitivity slice-PASEF-mediated global ubiquitinomics**; Martin Steger[1]; Uli Ohmayer[1]; Bjoern

Schwalb[1]; Jutta Fritz[1]; Vadim Demichev[2]; Henrik Daub[1]; *[1]NEOsphere Biotechnologies GmbH, Planegg, Germany; [2]Charité – Universitätsmedizin Berlin, Berlin, Germany*

TP 213 **LiP-MS combined with directDIA+ allows for highly specific drug target deconvolution**; Monika Pepelnjak[1]; Fabio Sabino[1]; Jaruschka Pecnik[1]; Roland Bruderer[1]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

TP 214 **Development of a robust covalent fragment screening platform using data independent acquisition (DIA) mass spectrometry**; Gregory K. Potts[1]; Alex Shannon[1]; Ryan A. McClure[1]; Adam Banlasan[1]; Hua Tang[1]; Violeta Marin[1]; Janice Lee[1]; Noah P. Tu[1]; Jon D. Williams[1]; Anil Vasudevan[1]; *[1]AbbVie, 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 Shyong[1]; Matthew T. Mazur[2]; Qian Huang[2]; Carl J. Balibar[2]; Weixun Wang[2]; *[1]Merck & Co. Inc., West Point, PA; [2]Merck & Co., Inc.,, West Point, PA*

TP 216 **Real-time batch LC-MS and NMR data processing and LIMS reporting for small molecule characterization**; Sarah Robinson[1]; Kewei Xu[1]; *[1]Genentech, Inc, South San Francisco, CA*

TP 217 **DrugMap: A Pan-Cancer Analysis of Protien Druggability**; Siwen Zhang[1]; Mariko Hara[1]; Harrison Byron Chong[1]; Liron Bar-Peled[1]; *[1]MGH, boston, MA*

TP 218 **A High Throughput QC Method for Assessing Serial Dilution Performance of Dose-Response Plates**; Lei Yang[1]; Mary Rimmer[1]; Kendall Billingsley[1]; Kaylee Bundy[1]; Mariana Santana Ponce[1]; Shalandus Garrett[1]; Chepyala Divyabharathi[1]; Yong Li[1]; Mitchell Sharnise[1]; Currier Duane[1]; Bryan Julianne[1]; Rankovic Zoran[1]; *[1]St. Jude Children's Research Hospital, Memphis, Tennessee*

TP 219 **Measuring Chromatography Column Effect on Mass Spec Feature Coelution and Deconvolvability**; Lizzie Spencer[1]; Laurel D. Wright[1]; Thomas Butler[1]; John T. Prince[1]; David Healey[1]; *[1]Enveda 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 Kirkwood[1]; James N Dodds[2]; Erin S Baker[2]; *[1]North Carolina State University, Raleigh, NC; [2]University 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 Rosnack[1]; Kari Organtini[1]; Henry Foddy[2]; Nicola Dreolin[2]; Stuart Adams[2]; Peter Hancock[2]; *[1]Waters Corporation, Milford, MA; [2]Waters 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 Kwon[1]; Seung-Min Lee[1]; Yeong-Jin Kim[1]; Yoon-Jeong Jeon[1]; Wenting Wang[1]; Jong-Su Seo[1]; Jong-Hwan Kim[1]; *[1]Environmental 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 Parry[1]; David A Weil[2]; Patrick Batoon[2]; Tarun Anumol[1]; *[1]Agilent Technologies, Wilmington; [2]Agilent 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 Passig[1]; Julian Schade[1, 2]; Ellen Iva Rosewig[1]; Lukas Alexander Anders[1]; Robert Irsig[3]; Sven Ehlert[3]; Andreas Walte[3]; Ralf Zimmermann[1]; *[1]Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; [2]University of Bundeswehr Munich, Faculty for Mechanical Engineering, Institute of Chemical and Environmental Engineering, Neubiberg, Germany; [3]Photonion GmbH, Schwerin, Germany*

TP 225 **High Resolution-MS uncovers new halocyclopentadiene disinfection by-products in drinking water**; Susan Richardson[1]; Jiafu Li[1, 2]; Md. Tareq Aziz[1]; Caroline Granger[1]; *[1]University of South Carolina, Columbia, SC; [2]Soochow University, Suzhou, China*

TP 226 **Evaluating detectability as LoD from the predicted ionization efficiency values for ESI+ and ESI-**; Amina Souihi[1]; Jonathan Martin[2]; Anneli Kruve[1]; *[1]Department of Environmental and Materials Chemistry, Stockholm University, Stockholm, Sweden; [2]Department 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 Abrell[1]; Osmar Luiz Moreira P F Menezes[1]; Kartika Srivastava[1]; Danielle Barrientes[1]; Jon Chorover[1]; Reyes Sierra Alvarez[1]; *[1]University 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 Fukuyama[1]; Kanako Sekimoto[1]; *[1]Yokohama City University, Yokohama-shi, Japan*

TP 229 **Mass Spectrometry tools for confident discrimination of different qualities of post-consumer recycled plastics**; Hania Khoury-Hollins[1]; Bryan Katzenmeyer[2]; Rachel J Sanig[3]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters corp, milford, MA; [3]Waters Corporation, Wilmslow, United Kingdom*

TP 230 **An ultra-high sensitivity analysis approach for detecting PFAS compounds in water sources**; Jianru Stahl-Zeng[1]; Bertram Nieland[2]; Jack Steed[3]; Abdessamad Chahbouni[4]; *[1]SCIEX, Darmstadt, Germany; [2]SCIEX, Darmstadt, Germany; [3]SCIEX, Macclesfield, United Kingdom; [4]Het Water Lab, J.W. Lucasweg 2 2031 BE Haarlem, Netherlands*

TP 231 **Comprehensive Analytical Workflow of PFAS Analysis in Aqueous Environmental Samples**; Ying Long[1]; Ana Ramos[1]; James Smalley[1]; Lam Leung[1]; *[1]Chemours, 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 Son[1]; Moonhee Park[2]; Young Hwan Kim[2]; Sunghwan Kim[1, 3]; *[1]Kyungpook National University, Daegu, South Korea; [2]Korea Basic Science Institute, Cheongju, South Korea; [3]Mass 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 Fatigante[1]; Sam Putnam[1]; Kushal Modi[1]; *[1]Bruker 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 Haddad[1]; Bruce D Quimby[1]; Anastasia A Andrianova[1]; Eric L Fausett[1]; *[1]Agilent 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 Dowling[1]; Sarah Prunty[1]; Katie Jensen[1]; Christine Picard[1]; Nicholas Manicke[1]; *[1]Indiana 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 Strattman[1]; Jacob Jalali[2]; Jesse Leonard[2]; Erasmus Cudjoe[3]; Marc R Elie[2]; *[1]PerkinElmer, Charlestown, RI; [2]PerkinElmer, Shelton , CT; [3]PerkinElmer Inc., Woodbridge, ON*

TP 237 **Evaluating Known and Novel PFAS in Firefighter Blood with Non-Targeted Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry Measurements**; Ashlee T Falls[1]; Anna Boatman[1]; Kaylie Kirkwood[2]; Heather M Stapleton[3]; Erin S Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]North Carolina State University, Raleigh, NC; [3]Duke 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. Beale[1]; Thomas Nguyen[1]; Utpal Bose[2]; Jordi Nelis[2]; Sally Stockwell[2]; James A. Broadbent[2]; Matthew C. Smith[3]; Andrew Bissett[3]; Gunjan Pandey[4]; Leon Court[4]; Rahul Rane[5]; Caitriona Walsh[4]; Nicholas Bourne[2]; Sandra Nilsson[6]; Viviana Gonzalez-Astudillo[7]; Christoph Braun[8]; Brenda Baddiley[8]; Stephanie Shaw[8]; Josh Llinas[9]; Duncan Limpus[8]; Suzanne Vardy[8]; *[1]CSIRO, Dutton Park, Australia; [2]CSIRO, St Lucia, Australia; [3]CSIRO, Hobart, Australia; [4]CSIRO, Canberra, Australia; [5]CSIRO, Parkville, Australia; [6]The University of Queensland, Woolloongabba, Australia; [7]The University of Queensland, Gatton, Australia; [8]Queensland Department of Environment and Science, Dutton Park, Australia; [9]Unusual Pets Veterinarian, Brisbane, Australia*

TP 239 **PY-GCMS analysis of microplastics in environmental samples using nitrogen as an alternative carrier gas**; Andy Sandy[1]; Evelyn Wang[2]; Ruth Marfil-Vega[2]; Yoshiyuki Okamura[2]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]Shimadzu Scientific Instrument, Columbia, Maryland*

TP 240 **Identification of a Serine-containing Microcystin by Thiol Derivatization and Specific MS/MS Neutral Losses**; Sanduni H Premathilaka[1]; Johnna A Birbeck[2]; Judy A Westrick[2]; Dragan Isailovic[1]; *[1]University of Toledo, Toledo, OH; [2]Wayne State University, Detroit , MI*

TP 241 **Characterizing the Isomeric Forms of PFASs in Biological Samples with UHPLC and Ion Mobility Mass Spectrometry**; Carrie A McDonough[1]; David Dukes[2]; Jennifer Marciano[2]; Emily Parry[3]; David A Weil[3]; Sheher Banu Mohsin[3]; *[1]Carnegie Mellon University, Pittsburgh, PA; [2]Stony Brook University, Stony Brook, NY; [3]Agilent Technologies, Santa Clara, CA*

TP 242 **Accurate mass library for PFAS analysis in environmental samples using high resolution GC/Q-TOF**; Sofia Nieto[1]; Matthew Giardina[1]; Luann Wong[2]; Gabrielle Black[2]; Thomas Young[2]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Department 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 Shih[1]; Chia-Yang Chen[1]; *[1]Institute 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**; Chongyean (shawn) Ehlers Cheang[1]; Cheng-Yu Weng[1]; Garret Couture[1]; Carlito B. Lebrilla[1]; *[1]University 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 Dong[1]; Xin Yang[1]; Ning Zhang[2]; Pei Chen[3]; Jianghao Sun[3]; James Harnly[3]; Mengliang Zhang[4]; *[1]Middle Tennesse State University, Murfreesboro, TN; [2]Fisk University, Nashville, TN; [3]USDA-ARS, Beltsivlle, MD; [4]MTSU, Murfreesboro, TN*

TP 246 **Intact mass characterization reveals novel post-translationally cleaved allergenic proteins from peanut**; Justin Marsh[1]; Danijela Apostolovic[2]; Govardus De Jong[3]; Stef J Koppelman[1]; Philip Johnson[1]; *[1]University of Nebraska Lincoln, Lincoln, NE; [2]Karolinska Institute, Solna, Sweden; [3]Wageningen 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 Vennard[1]; Nathan A. Meredith[1]; Michael Gray[1]; Sarah Maria[1]; Shay Phillips[1]; Lauren Brink[2]; Ruth Simmons[3]; *[1]Mead Johnson Nutrition, Evansville, IN; [2]Reckitt, Parsippany, NJ; [3]Reckitt, Slough, United Kingdom*

TP 248 **Quality Discrimination of Jasmine Tea using LC-Q/TOF Combined with Sensory Evaluation and Statistical Method**; Xinwei Feng[1]; Jason Li[1]; Nola Yu[1]; *[1]APTC, 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 Porcu[3]; Andrea Occhipinti[3]; Valentina Schiavo[1]; Claudio Medana[1]; *[1]University of Turin, Dipartimento di Biotecnologie Molecolari e Scienze per la Salute, Turin, Italy; [2]Biosfered S.R.L., Turin, Italy; [3]Abel Nutraceuticals, Turin, Italy*

TP 250 **Proteomics of Western Honeybees to Assess Colony Health**; Vincent Ricigliono[1]; Taylar Bell[2]; Ally Martin[1]; Fabrizio Donnarumma[2]; Kermit K. Murray[2]; *[1]USDA-ARS, Honey Bee Breeding, Genetics, and Physiology Research, Baton Rouge, Louisiana; [2]Louisiana 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 Bae[1]; Sun Koung Joung[1]; Hamin Choi[1]; Sang Beom Han[1]; *[1]Chung-Ang University, Seoul, South Korea*

TP 252 **High-resolution mass spectrometry (HRMS) method for determinate 43 per- and polyfluoroalkyl substances (PFAS) in vegetables**; Gui-Ru Xie[1]; HONG-JHANG Chen[1]; *[1]Institute 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 Daly[1]; Qianying Xu[2]; Si Cheng[3]; Lisa Reid[1]; Lee A Gethings[1]; Emma Marsden-Edwards[1]; E NC Mills[2, 4]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]University of Manchester, Manchester, United Kingdom; [3]Waters Corporation, Costa Mesa, CA; [4]University 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 Fornal[1]; Anna Stachniuk[1]; Magdalena Montowska[2]; Agata Sumara[1]; Alicja Trzpil[1]; *[1]Medical University of Lublin, Lublin, Poland; [2]Poznan 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 Bhuiyan[1]; Cristian D. Gutierrez Reyes[1]; Waziha Purba[1]; Andrew Bennett[1]; Sherifdeen Onigbinde[1]; Adeniyi Moyinoluwa[1]; Yehia Mechref[1]; *[1]Texas 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 Montaño-Pérez[1]; Guadalupe Yáñez-Ibarra[1]; Jorge-Luis Figueroa-Cordova[1, 3]; Cyndia-Azucena González-Arias[3]; *[1]Unidad Especializada en I+D+i Calidad de Alimentos y Productos Naturales, Centro Nayarita de Innovación y Transferencia de Tecnología A.C., Tepic, Mexico; [2]Unidad Académica de Ciencias Químico Biológicas y Farmacéuticas, Universidad Autónoma de Nayarit, Tepic, Mexico; [3]Laboratorio 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 Takahashi[1]; Mami Okamoto[1]; Yuta Miyazaki[1]; Yohei Arao[1]; Natsuyo Asano[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

TP 258 **Applications of LC-MS to analyze food-derived bioactive peptides: from food processing to simulated gastrointestinal digestion**; Yu-Ping Huang[1]; Fernanda Furlan Goncalves Dias[1]; Juliana Maria Leite Nobrega De Moura Bell[1]; Daniela Barile[1]; *[1]University 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 Stacy[1]; Anita Vinjamuri[1]; Carlito B. Lebrilla[1]; *[1]UC Davis, Davis, CA*

TP 260 **Onions, Garlic and FODMAPs: Characterization of Fructan Structure and Hydrolytic Effects of Microbial Inulinase Using LC-MS**; James G Farmar[1]; Justin L Guice[1]; Morgan D Hollins[1]; Kelly T Tinker[1]; Sean M Garvey[1]; *[1]BIO-CAT, Troy, VA*

TP 261 **Analysis of fatty acid content in rice by GC-MS/MS combined with metabolite database**; Yong Wang[1]; Jun Fan[2]; *[1]Shimadzu Enterprise Management (China) Co., Ltd, Beijing, China; [2]Shimadzu 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 Jones[1]; Jacqueline Michelle Chaparro[1]; Tyler J Richards[1]; Jessica Prenni[1]; *[1]Colorado 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 Mathai[1]; Cynthia (xinyi) Kuang[2]; Saketh Chemuru[3]; Daryl Giblin[2]; Michael L. Gross[3]; *[1]Emeritus - Sacred Heart College, Kochi, India; [2]Washington University in St.Louis, St.Louis, MO; [3]Washington 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. Defiglia[1]; Kristina Hakansson[1]; *[1]University of Michigan Ann-Arbor, Ann Arbor, MI*

TP 267 **Free OH Radicals Selectively Oxidize Heterocycles under APCI-MS**; Dmitry Eremin[1]; Shubhangi Aggarwal[1]; Valery Fokin[1]; *[1]University 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 Svingou[1]; Ri Wu[1]; Lukas Raphael Benzenberg[1]; Renato Zenobi[1]; *[1]ETH 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-Oviedo[1]; Robert Schiewe[2]; Harald Knorke[2]; Jonas Warneke[2, 3]; Julia Laskin[1]; *[1]Purdue University, West lafayette, Indiana; [2]Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, Leipzig University, Leipzig, Germany; [3]Leibniz Institute of Surface Engineering (IOM), Leipzig, Germany*

TP 270 **Use of Visualized Rayleigh Limit to Aid in Charge Detector Calibration**; David Hrabovsky[1]; Richard B. Cole[2]; *[1]Sorbonne Université, Faculté des Sciences et de l'Ingénierie, Paris, France; [2]Sorbonne 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 Porter[1]; Noah J Mismash[1]; Andrew J Arslanian[1, 2]; David V Dearden[1]; *[1]Brigham Young University, Provo, UT; [2]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH*

TP 272 **Factors Controlling Ion Yields in Droplet Assisted Ionization**; Jim Walker[1]; Kelvin Risby[1]; Oli Boswell[1]; Amaran Varma[1]; Joshua Harrison[1]; Bryan R Bzdek[1]; *[1]University of Bristol, Bristol, United Kingdom*

TP 273 **Bismuth-Mediated Capture of the Cysteine-Rich Dark Proteome in Mycobacteria**; Hannah A. Marietta[1]; C. Bruce Mousseau[1]; Matthew M. Champion[1]; *[1]University 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 Benzenberg[1]; Ri Wu[1]; Despoina Svingou[1]; Renato Zenobi[1]; *[1]ETH Zurich, Zurich, Switzerland*

TP 275 **Microdroplet Mass Spectrometry-based Method for Detecting Hemoglobin Adducts**; Hung-Hsiang Jen[1]; Kang-Yu Liu[1]; Shu-Hui Chen[1]; Chin-Ming Kuo[1]; Fung-Yu Chen[1]; *[1]National Cheng Kung University, Tainan, Taiwan*

TP 276 **Isotopocules of Oxyanions: A Journey from Ice Cores to Humans**; Cajetan Neubauer[1]; Kristýna Kantnerová[1]; Sebastian Kopf[1]; Andreas Hilkert[2]; *[1]University of Colorado Boulder, Boulder, CO; [2]Thermo 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 Stukalov[1]; Shadi Ferdosi[1]; Yingxiang Huang[1]; Moaraj Hasan[1]; Brittany Lee[1]; Asim Siddiqui[1]; Serafim Batzoglou[1]; Daniel Hornburg[1]; *[1]Seer Inc., Redwood City, CA*

TP 278 **High-efficiency survey of analytes enabled by modulated ion transfer and MS/MS analysis**; Xiaomin Fan[1]; Zheng Ouyang[1]; *[1]Department of Precision Instrument, Tsinghua University, Beijing, China*

TP 279 **Advances in molecular analysis at the nanoscale**; Thanh Loan Lai[1]; Dmitriy S. Verkhoturov[1]; Michael J. Eller[2]; Serge Della Negra[3]; Stanislav V. Verkhoturov[1]; Emile A. Schweikert[1]; *[1]Department of Chemistry, Texas A&M University, College Station, TX; [2]Department of Chemistry and Biochemistry, California State University Northridge, Northridge, CA; [3]University of Paris-Saclay, CNRS/IN2P3, IJCLab, Orsay, France*

TP 280 **Mucinase SmE enables improved glycoproteomic mapping of mucin-domain glycoproteins**; Alexandra Steigmeyer[1]; Joann Chongsaritsinsuk[1]; Keira E. Mahoney[1]; Taryn M. Lucas[1]; Deniz Ince[1]; Alexandria Battison[1]; Marie A. Hollenhorst[2]; D. Judy Shon[2]; Victor Attah[1]; Catherine Kwon[1]; Carolyn R. Bertozzi[2]; Stacy A. Malaker[1]; *[1]Yale University, New Haven, CT; [2]Stanford University, Stanford, CA*

TP 281 **Exposing the molecular heterogeneity of glycosylated biotherapeutics**; Luis F Schachner[1]; Christopher Mullen[2]; Wilson Phung[1]; Joshua Hinkle[2]; Michelle Irwin Beardsley[1]; Tracy Bentley[1]; Peter Day[1]; Christina Tsai[1]; Siddharth Sukumaran[1]; Tomasz Baginski[1]; Danielle Dicara[1]; Nicholas Agard[1]; Matthieu Masureel[1]; Joshua Gober[1]; Adel Elsohly[1]; John E.P. Syka[2]; Romain Huguet[2]; Michael T Marty[3]; Wendy Sandoval[1]; *[1]Genentech Inc, South San Francisco, CA; [2]Thermo Fisher Scientific, San Jose, California; [3]University of Arizona, Tucson, AZ*

TP 282 **Glycan-dependent Affinity Purification Mass Spectrometry (GAP-MS) provides novel insights into glycoprotein interaction network**; Yixuan (axe) Xie[1]; Xingyu Liu[1]; Siyu Chen[2]; Zongtao Lin[1]; Carlito B. Lebrilla[2]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO; [2]University 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 Li[1]; Chaoshuang Xia[2]; Haowei Tong[1]; Weiwei Wang[1]; Catherine

E. Costello[2]; Cheng Lin[2]; Juan Wei[1]; *[1]Shanghai Jiao Tong University, Shanghai, China; [2]Boston 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 Suttapitugsakul[1]; Yasuyuki Matsumoto[1]; Rajindra P Aryal[1]; Richard D Cummings[1]; *[1]Department 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 James[1]; Katelynn S. Zuercher[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

TP 286 **Optimization of Methods for Building Human Glycopeptide Libraries**; Yi Liu[1]; Meghan C. Burke[1]; Zachary C. Goecker[1]; Sergey L. Sheetlin[1]; Guanghui Wang[1]; Yuxue Liang[1]; Zheng Zhang[1]; Yuri A. Mirokhin[1]; Xiaoyu Yang[1]; Dmitrii V. Tchekhovskoi[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

TP 287 **N-Glycosylation Profile of EpCAM in Epithelial and Breast Cancer Cells**; Nicole M. Jenkinson[1]; Lauren R. DeVine[2, 3]; Caitlin M. Tressler[1]; Robert N. Cole[2, 3]; Kristine Glunde[1, 3, 4]; *[1]Russell H. Morgan Department of Radiology and Radiological Science, Division of Cancer Imaging Research, Johns Hopkins University School of Medicine, Baltimore, MD; [2]Mass Spectrometry and Proteomics Facility, Johns Hopkins University School of Medicine, Baltimore, MD; [3]Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD; [4]Sidney 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 Goecker[1]; Meghan C. Burke[1]; Concepcion A. Remoroza[1]; Yi Liu[1]; Yuri A. Mirokhin[1]; Sergey L. Sheetlin[2]; Dmitrii V. Tchekhovskoi[1]; Xiaoyu Yang[1]; Stephen E. Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]National 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 Wentao[1]; Song Hexing[2]; Luo Ji[3]; Chen Hongxu[2]; Guo Lihai[4]; *[1]sciex, guangzhou, China; [2]SCIEX, Beijing, China; [3]SCIEX, Shanghai, China; [4]SCIEX, Beijing, China*

TP 290 **One-step preparation of boric acid-riched hydrothermal spheres for N-glycopeptides analysis in preeclampsia serum**; Yinghua Yan[1]; Chuan-Fan Ding[1]; *[1]Ningbo 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. Burke[1]; Yi Liu[1]; Concepcion A. Remoroza[1]; Yuri A. Mirokhin[1]; Sergey Sheetlin[1]; Dmitrii V. Tchekhovskoi[1]; Guanghui Wang[1]; Xiaoyu Yang[1]; Stephen E. Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

TP 292 **Introducing the GlycoPaSER prototype for real-time N-glycopeptide identification on the PaSER platform**; Gad Armony[1]; Sven Brehmer[2]; Tharan Srikumar[3]; Lennard Pfenning[2]; Fokje Zijlstra[4]; Dennis Trede[2]; Gary Kruppa[5]; Dirk Lefeber[4, 6]; Alain Van Gool[4]; Hans Wessels[4]; *[1]Translational Metabolic Laboratory, Department of Laboratory Medicine, Radboud Institute for Molecular Life Sciences, RadboudUMC, Nijmegen, Netherlands; [2]Bruker Daltonics, Bremen, Germany; [3]Bruker Ltd, Milton, ON; [4]Translational Metabolic Laboratory, Department of Genetics, Radboud Institute for Molecular Life Sciences, RadboudUMC, Nijmegen, Netherlands; [5]Bruker S.R.O., Brno, Czech Republic; [6]Department 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 Wang[1]; Jakub Baudys[1]; Sarah H. Osman[2]; John R Barr[1]; *[1]Centers of Disease Control and Prevention (CDC), Atlanta, GA; [2]Centers 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 Bae[1]; Heeyoun Hwang[1, 2]; Young Ho Jeon[4]; Jin Young Kim[1, 2]; *[1]Korea Basic Science Institute, Cheoungju, South Korea; [2]Korea Research Institute of Bioscience and Biotechnology, Yuseong-gu, South Korea; [3]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; [4]Korea 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 Peng[1]; Jingzhi Zhao[1]; Ping Wu[1]; Gunagqing Chen[1]; Lukang Sun[1]; Jing Huang[1]; Jun Ma[1]; Wenting Li[1]; Baozhen Shan[1]; *[1]BaizhenBio Inc., shangahi, China*

TP 296 **Fragment ion triggered Parallel Accumulation SErial Fragmentation stepping for enhanced glycoproteomics data acquisition and beyond**; Gad Armony[1]; Michael Krause[2]; Pierre-Olivier Schmit[3]; Dennis Trede[2]; Gary Kruppa[4]; Dirk Lefeber[1, 5]; Alain Van Gool[1]; Hans Wessels[1]; *[1]Translational Metabolic Laboratory, Department of Laboratory Medicine, Radboud Institute for Molecular Life Sciences, RadboudUMC, Nijmegen, Netherlands; [2]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [3]Bruker Daltonique S.A., Wissembourg, France; [4]Bruker S.R.O., Brno, Czech Republic; [5]Department of Neurology, Donders Institute for Brain, Cognition and Behavior, RadboudUMC, Nijmegen, Netherlands*

TP 297 **Regulation of Protein N-linked Glycosylation Site Occupancy.**; Marium Khaleque[1]; Amanda S. Nouwens[1]; Benjamin L. Schulz[1]; *[1]The University of Queensland, Brisbane, Australia*

TP 298 **Quantitative glycoproteome analysis using a novel nanoparticle-based plasma proteomics workflow**; Shadi Ferdosi[1]; Moaraj Hasan[1]; Iman Mohtashemi[1]; Evan O'Brien[1]; Hongwei Wang[1]; Jian Wang[1]; Khatereh Motamedchaboki[1]; Harendra Guturu[1]; Daniel Hornburg[1]; *[1]Seer, 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 Alvarez[1]; Patrick Moreno[2]; Armin Oloumi[1]; Ryan Lee Schindler[1]; Qingwen Zhou[1]; Michelle Narciso[3]; Sheryl Joyce B. Grijaldo[3]; Ruel C. Nacario[3]; Gladys C. Completo[3]; Francisco M. Heralde III[2]; Carlito B. Lebrilla[1]; *[1]University of California Davis, Davis, CA; [2]Lung Center of the Philippines, Quezon City, Philippines; [3]University 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 Zeng[1]; Adam J Anthony[1]; Anu Sharma[2]; Jonathan C. Trinidad[1]; Subhadip Ghatak[2]; David E. Clemmer[1]; *[1]Indiana University Bloomington, Bloomington, IN; [2]Indiana University Purdue University Indianapolis, Indianapolis, IN*

TP 301 **Sialic acid isomer-targeted glycoprotein enrichment and proteomic characterization using bioorthogonal derivatization**; Hongxia Bai[1]; Collin McDowell[1]; Richard R. Drake[1]; *[1]Medical University of South Carolina, Charleston, SC*

TP 302 **Mass Spectrometry Analysis of N-linked Glycosylation on Influenza A(H3N2) Hemagglutinin and**

Neuraminidase from Inactivated Virus; Betlehem Mekonnen[1]; Irina Alymova[2]; Jakub Baudys[1]; Ian York[2]; Donxia Wang[1]; John R Barr[1]; *[1]CDC, Chamblee, GA; [2]CDC, Atlanta, GA*

TP 303 **Confident Identification of Multiply Glycosylated Peptides Using Hot Electron Capture Dissociation**; Margaret Downs[1]; Cheng Lin[1]; Chaoshuang Xia[1]; Athanasios Smyrnakis[2]; Dimitris Papanastasiou[2]; Joseph Zaia[1]; *[1]Boston University Chobanian and Avedisian School of Medicine, Boston, MA; [2]Fasmatech, NCSR Demokritos, Athens, Greece*

TP 304 **Comparative Glycomic and Glycoproteomic Analysis of Serum Exosomes Isolated Using Ultracentrifugation and Affinity-Based Method**; Mojibola O Fowowe[1]; Cristian D Gutierrez-Reyes[1]; Mojgan Atashi[1]; Sherifdeen Onigbinde[1]; Judith Nwaiwu[1]; Oluwatosin E Daramola[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

TP 305 **O-glycoproteomic mapping of amyloid precursor protein in Alzheimer's Disease**; Alexandria S. Battison[1]; Stacy A. Malaker[1]; *[1]Yale University, New Haven, CT*

TP 306 **Target Glycoproteomics and Proteomics Analysis with Parallel Reaction Monitoring (PRM) LC-MS/MS**; Moyinoluwa A Adeniyi[1]; Cristian D Gutierrez Reyes[1]; Mojgan Atashi[1]; Andrew I Bennett[1]; Sherifdeen Onigbinde[1]; Rogelio Najera Gonzalez[2]; David M Lubman[3]; Yehia Mechref[1]; *[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX; [2]Institute of Genomics for Crop Abiotic Stress Tolerance, Texas Tech University, Lubbock, TX; [3]Department of Surgery, The University of Michigan, Ann Arbor, MI*

TP 307 **The role of N-glycosylation in SARS-CoV-2 Spike protein binding specificity and kinetics**; Sarah H Osman[1]; Dongxia Wang[1]; Theodore R. Keppel[1]; John R Barr[1]; *[1]CDC, Chamblee, GA*

TP 308 **Isomeric Separation of α2,3/α2,6-linked 2-aminobenzamide (2AB)-labeled Sialoglycopeptides by C18-LC-MS/MS**; Peilin Jiang[1]; Yifan Huang[1]; Cristian D Gutierrez Reyes[1]; Jieqiang Zhong[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

TP 309 **Analysis of Mitochondria Glycomics and Glycoproteomics Isolated Using Different Enrichment Methods**; Judith Ijeoma Nwaiwu[1]; Oluwatosin E Daramola[1]; Mojgan Atashi[1]; Mojibola O Fowowe[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

TP 310 **LC-MS/MS Characterization of the N-glycosylation of Spike protein S1 Derived from 11 variants of SARS-CoV-2**; Cristian D Gutierrez Reyes[1]; Sherifdeen Onigbinde[1]; Andrew I. Bennett[1]; Akeem Sanni[1]; Peilin Jiang[1]; Oluwatosin E Daramola[1]; Mojgan Atashi[1]; Vishal Sandilya[1]; Mojibola O Fowowe[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, Texas*

TP 311 **Improved enrichment techniques for analysis of densely O-glycosylated domains from complex samples**; Keira Erol Mahoney[1]; Vincent Chang[1]; Taryn M. Lucas[1]; Stacy A. Malaker[1]; *[1]Yale University, New Haven, CT*

TP 312 **Comparison of the Relative Quantitation of N-linked Glycopeptides Using Different Chromatographic Separation Modes**; Mya M Brown[1]; Hoang Kim Ngan Thai[1]; Ron Orlando[1]; *[1]University of Georgia - Complex Carbohydrate Research Center, Athens, GA*

TP 313 **Development of an Automatic Three-Dimensional Mass Spectrometry Imaging System with Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI)**; Ying Xi[1]; Kevan Knizner[1]; Kenneth Garrard[1]; David Muddiman[1]; *[1]North Carolina State University, Raleigh, NC*

TP 314 **Achieving Sub Parts-Per-Million Mass Measurement Accuracy on an Orbitrap Mass Spectrometry Imaging Platform without Automatic Gain Control**; Russell R. Kibbe[1]; David C. Muddiman[1]; *[1]North Carolina State University, Raleigh, NC*

TP 315 **Super-resolution Expansion Mass Spectrometry Imaging**; Y. L. Winnie Hung[1]; Jianing Wang[1]; Chengyi Xie[1]; Zongwei Cai[1]; *[1]State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, China*

TP 316 **A simplified sample preparation strategy for high-throughput mass spectrometry imaging of spheroids**; Yuan Liu[1]; Jillian Johnson[1]; Hua Zhang[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

TP 317 **immuno-DESI-MSI Spatially Locates A Drug Target, Signaling Factors, and Enzymes on Tissue**; Xiaowei Song[1]; Richard N. Zare[1]; *[1]Stanford University, Stanford, CA*

TP 318 **Quantitative Biodistributions of Polymeric Nanocarriers and their Cargo via Metal-coded Mass Tag Approach**; Dheeraj K. Agrohia[1]; Ritabrita Goswami[1]; Teerapong Jantarat[1]; Yağız Anıl Çiçek[1]; Taewon Jeon[1]; Vincent M. Rotello[1]; Richard W. Vachet[1]; *[1]University of Massachusetts, Amherst, AMHERST, MA*

TP 319 **Improved Quantitative Imaging of Nanomaterials by LA-ICP-MS using a Novel Tissue Mimic Approach**; Teerapong Jantarat[1]; Joshua D Lauterbach[1]; Jeerapat Doungchawee[1]; Richard W. Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

TP 320 **RaMALDI imaging: a novel multimodal imaging workflow integrating Raman spectroscopic and MALDI mass spectrometry imaging of a single sample**; Jeong Hee Kim[1]; Ethan Yang[2]; Caitlin M Tressler[2]; Xinyi Elaine Shen[2]; Dalton R Brown[2]; Cole Johnson[2]; Ishan Barman[1]; Kristine Glunde[2]; *[1]Johns Hopkins University, Baltimore, MD; [2]Johns Hopkins University School of Medicine, Baltimore, MD*

TP 321 **Statistical Approach to System Suitability Testing (SST) for Mass Spectrometry Imaging by Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI)**; Olivia Dioli[1]; Hongxia Bai[1]; Emily Hector[1]; Kenneth P Garrard[1]; David C Muddiman[1]; *[1]North Carolina State University, Raleigh, NC*

TP 322 **Combining Multimodal Single Cell Imaging with Multiplexed Enzyme-based MALDI Mass Spectrometry Imaging for Translational Studies**; Jaclyn B Dunne[1]; Jake T. Griner[1]; Martin Romeo[1]; Carsten Krieg[1]; Mark Lim[2]; Anand S. Mehta[1]; Richard R. Drake[1]; Peggi M. Angel[1]; *[1]Medical University of South Carolina, Charleston, SC; [2]AmberGen, Inc., Billerica, MA*

TP 323 **Visualizing the Matrix: New Methods for Imaging the Distributions of Extracellular Matrix Proteins**; Akaansha Rampal[1]; Ngoc Vu[1]; Richard W. Vachet[1]; Shelly R. Peyton[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

TP 324 **High-coverage lipid C=C location isomers mass spectrometry imaging in biological tissues and tumor model**; Yanyan Chen[1]; Chengyi Xie[1]; Peisi Xie[1]; Jianing Wang[1]; Zongwei Cai[1]; *[1]State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, China*

TP 325 **Tissue treatment and post-ionization for mass spectrometry imaging of lipids: gains and losses**; Junhai Yang[1]; Austin B. Moyle[1]; Andrew Bowman[1]; Wayne Buck[1]; David S. Wagner[1]; *[1]AbbVie Inc., North Chicago, IL*

TP 326 **Robust tissue single-voxel collection and processing for spatially resolved proteomics**; Reta Birhanu Kitata[1]; Marija Velickovic[2]; Zhangyang Xu[1]; Rui Zhao[3]; Rosalie K. Chu[3]; Marda L. Jorgensen[4]; David Scholten[5]; Tao Liu[1]; Huiping Liu[5]; Clive H. Wasserfall[4]; Chia-Feng Tsai[1]; Tujin Shi[1]; *[1]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington 99354; [2]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; [3]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; [4]Department of Pathology, Immunology, and Laboratory Medicine, Diabetes Institute, College of Medicine, University of Florida, Gainesville, Florida 32611;*

[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. Sisley[1]; Oliver J. Hale[1]; Helen J. Cooper[1]; [1]*University of Birmingham, Birmingham, United Kingdom*

TP 328 **MALDI coupled with 193 nm ultraviolet photodissociation for the characterization of glycerophospholipids**; Melanie J Campbell[1]; Erin H. Seeley[1]; Jennifer S. Brodbelt[1]; [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 Gorman[1]; Michael Taylor[1]; Lia Tesfay[2]; Jessica K Lukowski[1]; Suzy Torti[2]; Christopher Anderton[1]; [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 Fagerquist[1]; Yanlin Shi[1]; [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 phytocompounds using MALDI-MSI**; Kevin J Zemaitis[1]; Vivian Lin[1]; Amirhossein H. Ahkami[1]; Tanya Winkler[1]; Robert Stanley[1]; Vimal Kumar Balasubramanian[1]; Christopher Anderton[1]; Dusan Velickovic[1]; [1]*PNNL, Richland, WA*

TP 332 **SpatialOMx analysis allows for the specific identification of lipid species paving the way for accurate flux analysis**; Sumankalai Ramachandran[1]; Beixi Wang[1]; Azad Eshghi[1]; Erica Forsberg[1]; Katherine Stumpo[1]; [1]*Bruker Daltonics, Billerica, MA*

TP 333 **MALDI-IHC-Guided In-Depth Spatial Proteomics: Targeted and Untargeted MSI Combined**; Britt S.R. Claes[1]; Kasper Krestensen[1]; Gargey Yagnik[2]; Andrej Grgic[1]; Christel Kuik[1]; Mark J. Lim[2]; Kenneth J. Rothschild[2]; Michiel Vandenbosch[1]; Ron M.a. Heeren[1]; [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 Kertesz[1]; Scott T. Retterer[1]; Muneeba Khalid[1]; John F. Cahill[1]; [1]*Oak Ridge National Laboratory, Oak Ridge, TN*

TP 335 **Mass spectrometry imaging of regioisomeric hormonal steroids**; Varun Vashneel Sharma[1]; Ingela Lanekoff[2]; [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 Wang[1]; Alexandria L. Sohn[1]; Juhi Samal[2]; Kevin Erning[2]; Tatiana Segura[2]; David C. Muddiman[1]; [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. Desyaterik[1]; Austin M. Jones[2]; Kara M. Rademeyer[2]; Mary Peace McRae[2]; Yury O. Tsybin[3]; Konstantin O. Nagornov[3]; Anton N. Kozhinov[3]; Angela D.M. Kashuba[1]; Elias P. Rosen[1]; [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 Bottomley[1]; Dr Jonathan Phillips[1]; Dr Philippa Hart[2]; [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 Tran[1]; William T. Andrews[1]; Eugene Moskovets[2]; Maureen A. Kane[1]; Jace W. Jones[1]; [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 Su[1]; John P. McGee[1]; Kenneth R Durbin[1]; Michael A. R. Hollas[1]; Thomas P. Conrads[2]; Ryan T. Fellers[1]; Jeannie M. Camarillo[1]; Jared O. Kafader[1]; Neil L. Kelleher[1]; [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. Schey[1]; Lee S Cantrell[2]; Zhen Wang[1]; [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 Addington[1]; Michael T Marty[1]; Anthony J Midey[2]; [1]*University of Arizona, Tuscon, Arizona;* [2]*Waters, Milford, MA*

TP 343 **Spatial molecular analysis of acute cocaine exposure**; Mariya Nezhyva[1]; Rami Yaka[2]; Per E. Andr´en[1]; Katy Margulis[2]; Erik T Jansson[1]; [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 Tomioka[1]; Ryota Tomioka[1]; Kosuke Ogata[1]; Issei Mori[2, 3]; Makoto Arita[2, 3]; Koshi Imami[2]; Naoyuki Sugiyama[1]; 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 Deininger[4]; Andra Pascale-Henke[4]; Konstantin Schwarze[4]; Lisa M. Butler[1, 2, 3]; Paul J. Trim[1, 3]; Marten F. Snel[1, 3]; Heiko Neuweger[4]; [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 Ellsworth[1]; Joshua L Fischer[2]; Ethan Yang[2]; Kasia Janota[2]; Richard E. Marinos[1]; [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-Haber[1]; Ethan Stancliffe[1]; Dhanalakshmi S. Anbukumar[1]; Blake E. Sells[1]; Jia Yi[1]; Kevin Cho[1]; Kayla Adkins-Travis[1]; Leah P. Shriver[1]; Gary J. Patti[1]; [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 Xu[1]; Rui Zhao[1]; Rosalie K. Chu[1]; Marda L. Jorgensen[2]; David Scholten[3]; Sarah M Williams[1]; Ying Zhu[1]; Daniel J Orton[1]; Tao Liu[1]; Huiping Liu[3]; Clive H. Wasserfall[2]; Chia-Feng Tsai[1]; Tujin Shi[1]; [1]*PNNL, Richland, WA;* [2]*University of Florida, Gainesville, FL;* [3]*Department of Pharmacology, Feinberg School of Medicine, Northwestern University, Chicago, Illinois 60611*

TP 349 **Using Native MS, Top-Down, and Bottom-Up Proteomics to Profile Regio-specific Protein Interactions on Tissue**; Sarah C Beno[1]; Raul A Villacob[1]; Neda Feizi Gilandeh[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

TP 350 **Spatial Multi-Omics Investigation of Prostate Cancer Heterogeneity using integrated spatially resolved lipidomics and transcriptomics**; Wanqiu Zhang[1, 2]; Xander Spotbeen[3]; Tassiani Sarretto[4, 5]; Fabio Socciarelli[6]; Sebastiaan Vanuytven[7, 8]; Jose Ignacio Alvira Larizgoitia[9, 10]; Sam Kint[7, 9]; David Wouters[9, 11]; Gabriele Partel[9]; Maria Mantas[12]; Thomas Gevaert[13]; Wout Devlies[14, 15]; Katy Vandereyken[7, 9]; Steven Joniau[14, 16]; Massimo Loda[17]; Bart De Moor[18]; Thierry Voet[7, 9]; Alejandro Sifrim[9, 11]; Shane Ellis[5, 19]; Marc Claesen[12]; Nico Verbeeck[12]; Johannes Swinnen[20]; *[1]STADIUS Center for Dynamical Systems, Signal Processing and Data Analytics, Department of Electrical Engineering (ESAT), KU Leuven, Leuven, Belgium; [2]Aspect Analytics NV, Genk, Belgium; [3]Laboratory of Lipid Metabolism and Cancer, KU Leuven and Leuven Cancer Institute (LKI), Leuven, Belgium; [4]Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; [5]Illawarra Health and Medical Research Institute, Wollongong, Australia; [6]Department of Pathology, Weill Cornell Medical College, New York, NY; [7]Laboratory of Reproductive Genomics, Department of Human Genetics, KU Leuven, Leuven, Belgium; [8]KU Leuven Institute for Single Cell Omics (LISCO), KU Leuven, Leuven, Belgium; [9]KU Leuven Institute for Single Cell Omics (LISCO), KU Leuven, Leuven, Belgium; [10]Laboratory of Multi-omic Integrative Bioinformatics, Department of Human Genetics, KU Leuven, Leuven, Belgium; [11]Laboratory of Multi-omic Integrative Bioinformatics, Department of Human Genetics, KU Leuven, Leuven, Belgium; [12]Aspect Analytics NV, Genk, Belgium; [13]Department of Urology, University Hospitals Leuven, Leuven, Belgium; [14]Department of Urology, University Hospitals Leuven, Leuven, Belgium; [15]Department of Development and Regeneration, KU Leuven, Leuven, Belgium; [16]Department of Development and Regeneration, KU Leuven, Leuven, Belgium; [17]Department of Pathology, Weill Cornell Medical College, New York, New York; [18]STADIUS Center for Dynamical Systems, Signal Processing and Data Analytics, Department of Electrical Engineering (ESAT), KU Leuven, Leuven, Belgium; [19]Molecular Horizons and School of Chemistry and Molecular Bioscience, University of Wollongong, Wollongong, Australia; [20]Laboratory 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 Dahl[1]; Md Amir Hossen[2]; *[1]Shimadzu, Columbia, MD; [2]Shimadzu 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 West[3]; Katherine A. Stumpo[3]; Young Ah Goo[1, 2]; *[1]Mass Spectrometry Technology Access Center (MTAC@MGI), St Louis, MO; [2]Washington University School of Medicine, St. Louis, MO; [3]Bruker Daltonics GmbH & Co.KG, Bremen, Germany*

TP 353 **Single-voxel spatial proteomics for resolving 14 ROIs across the whole mouse brain tissue section**; Zhangyang Xu[1]; Reta Birhanu Kitata[1]; Rosalie K. Chu[1]; Rui Zhao[2]; Le Z. Day[1]; Matthew J Gaffrey[1]; Tao Liu[1]; Song-Lin Ding[3]; Tong Zhang[1]; Tujin Shi[1]; *[1]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington 99354; [2]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; [3]Allen 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 Lardenoije[3]; Lukasz G Migas[4]; Morad Malek[1, 5]; Haichun Yang[6, 7]; Agnes B Fogo[6, 7, 8]; Raf Van De Plas[1, 2, 4]; Joana P Gonçalves[3]; Richard M Caprioli[1, 2, 9, 10, 11]; Jeffrey M Spraggins[1, 2, 5, 11]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Biochemistry, Vanderbilt University, Nashville, TN; [3]Department of Intelligent Systems, Delft University of Technology, Delft, South Holland; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [6]Department of Pathology, Microbiology and immunology, Vanderbilt University, Nashville, TN; [7]Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; [8]Division of Nephrology, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; [9]Department of Medicine, Vanderbilt University, Nashville, TN; [10]Department of Pharmacology, Vanderbilt University, Nashville, TN; [11]Department of Chemistry, Vanderbilt University, Nashville, TN*

TP 355 **Maximizing Data Coverage with Sequential Imaging of a Single Tissue Section**; Erin H Seeley[1]; Edwin Escobar[1]; Jennifer S Brodbelt[1]; *[1]University 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 Lardenoije[5]; 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 Gonçalves[5]; Jeffrey M Spraggins[1, 2, 3, 4]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Chemistry, Vanderbilt University, Nashville, TN; [5]Department of Intelligent Systems, Delft University of Technology, Delft, Netherlands; [6]Delft 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 Zhang[2]; Shoba Sharma[1]; Aaron Ruiz[1]; Fabio C Tucci[3]; Kumar Sharma[2]; *[1]SygnaMap, Inc., San Antonio, TX; [2]Center for Precision Medicine, UT Health San Antonio, San Antonio, Texas; [3]Epigen 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 Huang[1]; Hua Zhang[2]; Manish Patankar[3]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Department 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 Levy[1]; Vignesh Venkataramani[2]; Laura Sanchez[3]; Lydia Kisley[2]; *[1]University of California Santa Cruz, Santa Cruz, CA; [2]Department of Biophysics and Chemistry, Case Western Reserve University, Cleveland, OH; [3]University of California, Santa Cruz, Santa Cruz, CA*

TP 360 **Updates to FragPipe computational platform: new capabilities, tools, and workflows**; Fengchao Yu[1]; Daniel Polasky[1]; Guo Ci Teo[1]; Felipe Da Veiga Leprevost[1]; Kai Li[1]; Kevin L Yang[1]; Yi Hsiao[1]; Ginny Xiaohe Li[1]; Carolina Rojas Ramirez[1]; Sarah Haynes[1]; Daniel J Geiszler[1]; Hui-Yin

Chang[1, 2]; Dmitry Avtonomov[1]; Andy T. Kong[1]; Alexey I Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI; [2]National Central University, Taoyuan, Taiwan*

TP 361 **Localized Microsampling of Formalin Fixed Paraffin Embedded Tissue for Proteomics**; Blessing Chisom Egbejiogu[1]; Kermit K. Murray[1]; *[1]Louisiana 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 Bindra[1]; Udayan Das[1]; James Pesavento[1]; *[1]Saint 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 Chen[1]; Yong Zang[2]; Xiaowen Liu[3, 4]; *[1]Department of BioHealth Informatics, Indiana University-Purdue University Indianapolis, Indianapolis, IN; [2]Department of Biostatics and Health Data Sciences, Indiana University School of Medicine, Indianapolis, IN; [3]Deming Department of Medicine, Tulane University, New Orleans, LA; [4]Tulane 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 Fu[1]; Huan Sun[1]; Zhiping Wu[1]; Zhen Wang[1]; Suresh Poudel[1]; Zuo-Fei Yuan[1]; Karthik Vadambacheri Manian[1]; Xusheng Wang[1]; Junmin Peng[1]; *[1]St. Jude Children's Research Hospital, Memphis, TN*

TP 365 **Optimization of DIA proteomics workflows using ground truth data simulated with Synthedia**; Michael G Leeming[1]; Ching-Seng Ang[1]; Shuai Nie[1]; Swati Varshney[1]; Nicholas A Williamson[1]; *[1]The University of Melbourne, Melbourne, Australia*

TP 366 **Highly sensitive and scalable timsTOF Pro data analysis with MaxDIA 2.0**; Juan L Restrepo-López[1]; Dmitry Alexeev[1]; Carlo De Nart[1]; Juergen Cox[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany*

TP 367 **FilterFASTA: a Tool for Generating Keyword Based Bespoke Cross-Organism FASTA's for Proteomics**; John Chlystek[1]; Jonathan Le[1]; Jonathan Katz[1, 2]; *[1]Lawrence J. Ellison Institute for Transformative Medicine, Los Angeles, CA; [2]USC, Los Angeles, CA*

TP 368 **An adaptive model for the protein inference problem**; Emile Benoist[1]; Guillaume Fertin[1]; Géraldine Jean[1]; *[1]LS2N, Nantes Université, Nantes Cedex 3, France*

TP 369 **Bayesian Confidence Intervals for Absolute Protein Quantification**; Chirag K Kumar[1]; Meera Gupta[1]; Donovan Cassidy-Nolan[1]; Arjuna Subramanian[1]; Vyas Pujari[1]; Martin Wuehr[1]; *[1]Lewis-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. McFarland[1]; Sara M. Handy[1]; Elizabeth Hunter[1]; Christine H. Parker[1]; Ann M. Knolhoff[1]; *[1]FDA-CFSAN, College Park, MD*

TP 371 **A Streamlined Data Analysis Workflow for Enhanced New Peak Detection (NPD) in the Multi-Attribute Method (MAM)**; Maurizio Bronzetti[1]; Aude Tartiere[1]; Stephen Kok[1]; Amy Claydon[2]; Arnd Brandenburg[3]; *[1]Genedata Inc., San Francisco, CA; [2]Genedata Ltd, Cambridge, United Kingdom; [3]Genedata 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 Lavanant[1]; Carlos Afonso[1, 2]; *[1]Normandie Univ, UNIROUEN, INSA Rouen, CNRS, COBRA, 76000 Rouen, France., Mont Saint Aignan, France; [2]International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harfleur, France; [3]TotalEnergies OneTech R&D, TotalEnergies Research & Technology, Gonfreville, France; [4]TotalEnergies Marketing Services, Research Center, Solaize, France; [5]Joint 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 Liu[2]; Yabing Zhu[3]; Zhe Ren[2]; Siqi Liu[1, 2]; *[1]College of Life Science, University of Chinese Academy of Sciences, Beijing, China; [2]Center of Proteomic Analysis, BGI Life Science Research Institute, Shenzhen, China; [3]BGI Genomics, BGIShenzhen, Shenzhen, China*

TP 374 **Fast Component Identification & Automated Well-to-Data Connectivity for High Throughput Workflows**; Richard Lee[1]; Nikki Dare[1]; Rostislav Pol[1]; Sofya Chudova[1]; Nikolay Malashchenok[1]; *[1]ACD/Labs, Toronto, ON*

TP 375 **Streamlining Metadata Capture for Mass Spectrometry Experiments: towards FAIR Omics metadata across R&D**; Benjamin Pullman[1]; Norelle C. Wildburger[1]; Matthew Glover[1]; Raghothama Chaerkady[1]; Jana Zecha[1]; Sri Vishnu Vardhan Deevi[2]; Lisa H Cazares[1]; Sonja Hess[1]; Stewart MacArthur[2]; Sebastian Wasilewski[2]; *[1]AstraZeneca, Gaithersburg, MD; [2]AstraZeneca, Cambridge, United Kingdom*

TP 376 **Creating a data analysis pipeline for producing high-quality glycopeptide mass spectral libraries**; Sergey Sheetlin[1]; Yuri A. Mirokhin[1]; Guanghui Wang[1]; Xiaoyu Yang[1]; Concepcion Remoroza[1]; Yi Liu[1]; Xinjian Yan[1]; Dmitrii V. Tchekhovskoi[1]; Zachary C. Goecker[1]; Meghan C. Burke[1]; Stephen E. Stein[1]; *[1]NIST, 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 Liu[3]; Brett Larsen[3]; Geoffrey Hesketh[4]; Payman Samavarchi Tehrani[3]; Hala Abdouni[3]; Anne-Claude Gingras[1, 3]; Hannes Röst[1, 2]; *[1]University of Toronto, Toronto, ON; [2]Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON; [3]Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto, ON; [4]Dalhousie University, Halifax, NS*

TP 378 **Workflomics: Facilitating the "Great Bake Off" of Computational Workflows for the Analysis of Mass Spectrometry Data**; Vedran Kasalica[1]; Nauman Ahmed[1]; Rob J Marissen[2]; Saskia Hiltemann[3]; Pratik Jagtap[4]; Melanie Föll[5]; Hervé Ménager[6]; Matúš Kalaš[7]; Michael R. Crusoe[8, 9]; Ana Redondo[10]; Salvador Capella-Gutierrez[10]; Veit Schwämmle[11]; Anna-Lena Lamprecht[12]; Magnus Palmblad[2]; *[1]Netherlands eScience Center, Amsterdam, Netherlands; [2]Leiden University Medical Center, Leiden, Netherlands; [3]Erasmus Medical Center Rotterdam, Rotterdam, Netherlands; [4]University of Minnesota, Minneapolis, MN; [5]University of Freiburg, Freiburg, Germany; [6]Institute Pasteur, Paris, France; [7]University of Bergen, Bergen, Norway; [8]Vrije Universiteit Amsterdam, Amsterdam, Netherlands; [9]Forschungszentrum Jülich, Jülich, Germany; [10]Barcelona Supercomputing Center, Barcelona, Spain; [11]University of Southern Denmark, Odense, Denmark; [12]University of Potsdam, Potsdam, Germany*

TP 379 **MassKit: A Flexible and High Performance API for Mass Spectrometry**; Douglas Slotta[1]; Lewis Y. Geer[1]; *[1]NIST, Gaithersburg, MD*

TP 380 **Chimerys server: deploying the power of the cloud in your basement**; Markus Schneider[1]; Tobias Schmidt[1]; Daniel P. Zolg[1]; Siegfried Gessulat[1]; Florian Seefried[1]; Samia Ben Fredj[1]; Martin Heinrich Frejno[1]; *[1]MSAID 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 Srikumar[1]; Mark Rocco Condina[2];

Jonathan Krieger[1]; Giuseppe Infusini[2]; Brad Green[2]; Paula Burton Ngov[2]; Aaron Triantafyllidis[2]; Saima Ahmed[3, 4]; Arthur Viode[3, 4]; Patrick Van Zalm[3, 4]; Sven Brehmer[5]; Dennis Trede[5]; Christopher Adams[6]; Judith Steen[3, 4]; Shibani S. Mukerji[4]; Hanno Steen[3, 4]; Andrew Ian Webb[2]; *[1]Bruker Ltd., Milton, ON; [2]Mass Dynamics, Melbourne, Australia; [3]Boston Childrens Hospital, Boston, MA; [4]Harvard Medical School, Boston, MA; [5]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [6]Bruker Scientific, San Jose, CA*

TP 382 **prolfquapp: Streamlining Protein Differential Expression Analysis in Core Facilities**; Witold E. Wolski[1]; Jonas Grossmann[1]; Paolo Nanni[1]; Bernd Roschitzki[1]; Claudia Fortes[1]; Christian Panse[1]; Ralph Schlapbach[1]; *[1]Functional 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 Guergues[1]; Jonathan R Krieger[2]; John M Koomen[3]; Sameer Varma[1]; Stanley Stevens Jr. [1]; *[1]University of South Florida, Tampa, FL; [2]Bruker Ltd., Milton, ON; [3]Moffitt 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 Harvey[1]; Adi M Kulkarni[2]; Kristina Srzentic[3]; Marshall Bern[1]; Ignat Shilov[1]; St. John Skilton[1]; Kate Yu[2]; *[1]Protein Metrics, LLC, Cupertino, CA; [2]908 Devices, Inc., Boston, MA; [3]ThermoFisher Scientific, San Jose, CA*

TP 385 **Tidyproteomics: An open-source R package and data object for quantitative proteomics post analysis and visualization**; Jeffrey J. Jones[1]; Brett Lomenick[1]; Ting-You Wang[1]; Tsui-Fen Chou[1]; *[1]Caltech, Pasadena, CA*

TP 386 **Centralized metabolomics reference database for standardized small molecule mass spectrometry data analysis**; Anastasiya V. Prymolenna[1]; Jordan M. Rabus[1]; Montana L. Smith[1]; Natasha N. Arokium-Christian[1]; Priscila M. Lalli[1]; Chaevien S. Clendinen[1]; Nathalie Munoz Munoz[1]; William R. Kew[1]; Young-Mo Kim[1]; Lee Ann McCrue[1]; Yuri E. Corilo[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TP 387 **MiCId GUI, a fast Microorganism Classification and Identification workflow with accurate statistics and high recall**; Aleksey Y Ogurtsov[1]; Gelio Alves[1]; Yi-Kuo Yu[1]; *[1]CBB NCBI NLM NIH, Bethesda, MD*

TP 388 **Open Platform for Automated Backup, Processing and Visualization of MS-based Omics Data**; Xiaofeng Xie[1]; Thy Truong[1]; Kei Webber[1]; Yiran Liang[1]; Madisyn Johnston[1]; Samuel H Payne[1]; Ryan Kelly[1]; *[1]Brigham Young University, Provo, UT*

TP 389 **MassIVE: adding value to all public data through automatic indexing and query tools**; Jeremy Carver[1]; Nuno Bandeira[1]; *[1]UCSD, La Jolla, CA*

TP 390 **Proteomics Standards Initiative (PSI) proposed peak annotation format (mzPAF) and spectral library format (mzSpecLib) standards**; Henry Lam[1]; Tytus D. Mak[2]; Joshua A. Klein[3]; Wout Bittremieux[4]; Ralf Gabriels[5]; Yasset Perez-Riverol[6]; Tim Van Den Bossche[5]; Andrew R Jones[7]; Pierre-Alain Binz[8]; Shin Kawano[9]; Luis Mendoza[10]; Nuno Bandeira[11]; Jeremy Carver[11]; Benjamin Pullman[11]; Zhi Sun[10]; Nils Hoffmann[12]; Jim Shofstahl[13]; Yunping Zhu[14]; Helge Hecht[15]; Eric Deutsch[10]; Juan Antonio Vizcaino[16]; *[1]Hong Kong University of Science and Technology, Hong Kong, Hong Kong; [2]National Institute of Standards and Technology, Gaithersburg, MD; [3]Boston University School of Medicine, Boston, MA; [4]University of Antwerp, Antwerpen, Belgium; [5]VIB-UGent Center for Medical Biotechnology, Gent, Belgium; [6]European Molecular Biology Laboratory (EMBL), Heidelberg, Germany; [7]University of Liverpool, Liverpool, United Kingdom; [8]Lausanne University Hospital, Lausanne, Switzerland; [9]Kitasato University, Kitasato, Japan; [10]Institute for Systems Biology, Seattle, WA; [11]University of California San Diego, San Diego, CA; [12]Forschungszentrum Jülich, Jülich, Germany; [13]Thermo Fisher Scientific, San Jose, California; [14]National Center for Protein Sciences (The PHOENIX Center, Beijing), Beijing, China; [15]Masaryk University, Brno, Czech Republic; [16]European Molecular Biology Laboratory, Heidelberg, Germany*

TP 391 **ADAP informatics for untargeted mass spectrometry-based metabolomics and exposomics big data**; Aleksandr Smirnov[1]; Joel Hall[1]; Toan Nguyen[1]; Yunfei Liao[2]; Daisy Brumit[1]; Yuanyuan Li[3]; Blake Rushing[3]; Susan McRitchie[3]; Radha Krishna Balaji[1]; Komal Madamwar[1]; Varun Suresh[1]; Shanmukh Gorle[2]; Anantnaval Gaikwad[1]; Steffy Roselina Eben Judson[1]; Susan Sumner[3]; Xiuxia Du[2]; *[1]University of North Carolina at Charlotte, Charlotte, North Carolina; [2]University of North Carolinat at Charlotte, Charlotte, NC; [3]University 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 Lee[1]; Jinlyung Choi[1]; Sara Nouri Golmaei[1]; Yuntao Hu[1]; Sai Ramaswamy[1]; Dijana Vitko[1]; Wan-Fang Chou[1]; Megan Mora[1]; Jessica Chan[1]; Mark Marispini[1]; Benjamin Ta[1]; Peter Spiro[1]; Hoda Malekpour[1]; Ajinkya Kokate[1]; Robert Zawada[1]; Bruce Wilcox[1]; Philip Ma[1]; Chinmay Belthangady[1]; Manway Liu[1]; *[1]PrognomiQ 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 Bulloch[1]; Han-Yin Yang[1]; Aman Makaju[2]; Ishwar N Kohale[1]; Bradford Gibson[1]; *[1]Amgen, South San Francisco, CA; [2]Amgen, 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. Lorenz[1]; Michael D. Thatcher[1]; Megan E. Sterling[1]; *[1]Food and Drug Administration, Office of Regulatory Affairs, Forensic Chemistry Center, Cincinnati, OH*

TP 395 **Portable MALDI-TOF Mass Spectrometer for Bioaerosol Detection**; Vadym Berkout[1]; Stuart Collymore[1]; Scott Ecelberger[1]; Max Cetta[1]; Lara Moore[1]; Caroline Haddaway[1]; Wayne Bryden[1]; Mike McLaughlin[1]; *[1]Zeteo Tech, Inc., Sykesville, MD*

TP 396 **Technology Advancements for the Extraterrestrial Molecular Indicators of Life Investigation (EMILI) Capillary Electrophoresis Electrospray Ionization Mass Spectrometer**; Desmond A. Kaplan[1, 2]; Maria Fernanda Mora[3]; Tomas Drevinskas[3]; Marco E. Castillo[1, 4]; Ryan M. Danell[1, 5]; Jacob D Graham[1]; Friso Van Amerom[1, 6]; Xiang Li[1]; Andrej Grubisic[1]; Bethany P Theiling[1]; Aaron C Noell[7]; Antonio J Ricco[8]; William B Brinckerhoff[1]; Peter A Willis[3]; *[1]National Aeronautics and Space Administration Goddard Space Flight Center, Greenbelt, MD; [2]KapScience LLC, TEWKSBURY, MA; [3]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA; [4]Aerodyne, Cape Canaveral, FL; [5]Danell Consulting, Winterville, NC; [6]Mini-Mass Consulting, Inc, Hyattesville, MD; [7]National Aeronautics and Space Administration Jet Propulsion Laboratory, Pasadena, CA; [8]National 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 Li[2]; Marco E. Castillo[2, 3]; Ryan M. Danell[2, 4]; Desmond A. Kaplan[2, 5]; Andrej Grubisic[2]; William B. Brinckerhoff[2]; And The Moma Team[6]; *[1]Mini-Mass Consulting, Inc, Hyattsville, MD; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]ASES, Beltsville, MD; [4]Danell Consulting, Winterville, NC; [5]KapScience LLC, TEWKSBURY, MA; [6]Max-Planck-Institut für Sonnensystemforschung, Göttingen, Germany*

TP 398 **Amino Acid Quantitation of Cell Culture Media Matrices via an Integrated CE-MS Analyzer**; Ji Young L Anderson[1]; William Morgan-Evans[2]; Bethany Kerr[2]; Kenion H Blakeman[1]; Milla Neffling[1]; Graziella Piras[1]; *[1]908 Devices, Inc., Boston, MA; [2]CPI Innovation Services Ltd., Darlington, United Kingdom*

TP 399 **Prototype Development of a Digital Linear Ion Trap based Portable GCMS for VOCs Analysis**; Chenzhang Zhu[1]; Lin Liu[1]; Hongbing Cheng[1]; Yulei Hu[1]; Xinfeng Zhou[1]; Wenjian Sun[1]; *[1]Shimadzu Research Laboratory, Shanghai, China*

TP 400 **Interfacing and Characterizing Portable HPLC Interfaced with Miniature Ion Trap Mass Spectrometer**; Vladimir M Doroshenko[1]; Victor Laiko[1]; Venkateswara Panchagnula[1]; Matthew Morse[2]; John Stimus[2]; *[1]MassTech, Inc., Columbia, MD; [2]Axcend LLC, Provo, UT*

TP 401 **Intelligent Miniature Mass Spectrometry System for Point-of-Care Analysis**; Bin Jiao[1]; Yikun Liu[1]; Xinwei Liu[1]; Jiexun Bu[2]; Wenpng Zhang[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China; [2]PURSPEC Technology (Beijing) Ltd., Beijing, China*

TP 402 **Portable Mass Spectrometer for air born particle detection**; Chung-Hsuan Chen[1]; Chun-Jen Hsiao Hsiao[2]; Ju-Yao Chang[1]; Jung-Lee Lin[2]; Abdil Ozdemir[3]; *[1]National Sun Yat-Sen University, Kaohsiung City, Taiwan; [2]Academia Sinica, Taipei, Taiwan; [3]Sakarya University, Sakarya, Turkey*

TP 403 **Modification of a Thermo LTQ-XL to Enable Automatic Gain Control and On-Demand 2D-MS/MS**; Eric T Dziekonski[1]; R. Graham Cooks[1]; *[1]Purdue University, WEST LAFAYETTE, IN*

TP 404 **Theory and Performance of a Novel High-Resolution Mass Analyzer**; Hamish Stewart[1]; Christian Hock[1]; Dmitry Grinfeld[1]; Matthias Biel[1]; Philipp Cochems[1]; Alexander Wagner[1]; Wilko Balschun[1]; Alexander Makarov[1]; *[1]Thermo 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 Richardson[1]; Martin Green[1]; David Langridge[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

TP 406 **Analysis of Megadalton ions using a novel dual sector Charge Detection Mass Spectrometer (CDMS)** ; John B Hoyes[1]; Dimitris Papanastasiou[2]; Alexandros Lekkas[2]; Yury Tsybin[3]; Anton Kozhinov[3]; Igor Filippov[4]; *[1]TrueMass, Rowarth, United Kingdom; [2]Fasmatech, NCSR Demokritos, Athens, Greece; [3]Spectroswiss, Lausanne, Switzerland; [4]MSCUBE 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 Chakravorty[1]; Elizabeth Groetsema[1]; Fatima Olayemi Obe[1]; Gordon Anderson[2]; Peter T. A. Reilly[1]; *[1]Washington State University, Pullman, WA; [2]GAA Custom Electronics, LLC, Benton City, WA*

TP 408 **Developing the trap/filter/eject methodology for isolation and mass analysis in higher stability zones**; Elizabeth Groetsema[1]; Sumeet Chakravorty[1]; Fatima Olayemi Obe[1]; Gordon Anderson[2]; Peter T. A. Reilly[1]; *[1]Washington State University, Pullman, WA; [2]GAA Custom Electronics, LLC, Benton City, WA*

TP 409 **Genetic algorithm parallel optimization high-resolution planar electrostatic ion trap mass analyzer**; Weimin Wang[1]; Fuxing Xu[1]; Li Ding[1]; Chuan-Fan Ding[1]; *[1]Ningbo University, Ningbo, China*

TP 410 **Integration of a SLIM-based High Resolution Ion Mobility Prototype with an Orbitrap Mass Spectrometer**; Alan A McKenzie-Coe[1]; Liulin Deng[2]; Brian Adamson[3]; Kyle L. Fort[4]; Eloy R Wouters[3]; Gordon A Anderson[5]; Lee Earley[6]; Jean-Jacques Dunyach[7]; Daniel Debord[2]; Alexander A Makarov[4]; *[1]MOBILion Systems, Inc., Chadds Ford, PA; [2]MOBILion Systems, Inc, Chadds Ford, PA; [3]Thermo Fisher Scientific, San Jose, California; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [5]GAA Custom Electronics, LLC, Benton City, WA; [6]Thermo Fisher Scientific, Boston, MA; [7]ThermoFisher 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 Weitz[1]; Bryson Gibbons[1]; Rosalie K. Chu[1]; James J Moran[1, 2]; Ljiljana Pasa-Tolic[1]; Amirhossein H. Ahkami[1]; Kirsten S. Hofmockel[1]; Janet K. Janssen[1]; Mary S Lipton[1]; *[1]Battelle Pacific Northwest National Laboratories, Richland, WA; [2]Michigan State University, East Lansing, MI*

TP 412 **A Novel Digital Waveform Generator for Creating High Resolution, Low Jitter, Rectangular Waveforms**; Gordon Anderson[1]; Sumeet Chakravorty[2]; Fatima Obe[2]; Elizabeth Groetsema[2]; Peter T. A. Reilly[2]; *[1]GAA Custom Electronics, LLC, Benton City, WA; [2]Washington 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. Reilly[1]; Sumeet S Chakravorty[1]; Fatima Olayemi Obe[1]; Elizabeth Groetsema[1]; Gordon Anderson[2]; *[1]Washington State University, Pullman, WA; [2]GAA Custom Electronics, LLC, Benton City, WA*

TP 414 **Using a branched RF-ion trap to combine EAD, ultraviolet-photodissociation (UVPD) and CID fragmentation**; Mircea Guna[1]; Pavel Ryumin[1]; Anjali Chelur[1]; Nick Albeanu[1]; Takashi Baba[1]; Yves Le Blanc[2]; *[1]SCIEX, Concord, ON; [2]SCIEX, Concord, On, ON*

TP 415 **Improving the Efficiency of Isolation of Native Protein Complexes by a Digital Mass Filter**; Robert Schrader[1]; David Russell[1]; *[1]Texas 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 Bensaoula[1]; Patrick Sturm[1]; Janos Metzger[1]; Carsten Stoemer[1]; Chia-Yu Tzou[1]; Georgios Papadopoulos[1]; Caroline Hain[2]; Thomas Nelis[2]; Jonathan Thomet[3]; *[1]Tofwerk AG, Thun, Switzerland; [2]Berner Fachhochschule BFH, Biel, Switzerland; [3]Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland*

TP 417 **Application of the Digital Tandem Mass Filter in Native Spray Analysis of Proteins**; Fatima Olayemi Obe[1]; Sumeet S. Chakravorty[1]; Elizabeth Groetsema[1]; Gordon A. Anderson[2]; Peter T. A. Reilly[1]; *[1]Washington State University, Pullman, WA; [2]GAA Custom Electronics, LLC, Benton City, WA*

TP 418 **Real-Time Optimization of Ultra-High Resolution in Charge Detection Mass Spectrometry**; David Reitenbach[1]; Daniel Y Botamanenko[2]; Martin F. Jarrold[2]; *[1]Indiana University, Bloomington, IN; [2]Indiana 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 Shih[1]; Patrick J Faustino[1]; Thomas O'Connor[1]; Xiaoming Xu[1]; Jinhui Zhang[1]; *[1]Food and Drug Administration, Silver Spring, MD*

TP 420 **Trapped Ion Mobility Spectrometry (tims) Facilitates Lipid and Metabolite Identification in MALDI Mass Spectrometry Imaging**; Min Liu[1]; Carolina Cruz Cepeda[1]; John M Koomen[1]; *[1]Moffitt Cancer Center, Tampa, FL*

TP 421 **Developing tandem mass spectrometry file structures for ion mobility spectrometry workflows**; Bryson Gibbons[1]; Sarah Stow[2]; Ruwan T Kurulugama[2]; Lauren Royer[3]; Daniel Debord[3]; John C Fjeldsted[2]; Richard D. Smith[1]; Aivett Bilbao[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Agilent Technologies, Santa Clara, CA; [3]MOBILion Systems, Inc., Chadds Ford, PA*

TP 422 **Implementation of a Highly Modular Structures for Lossless Ion Manipulations-Time-of-Flight Mass**

Spectrometry Platform; Zackary R Kinlein[1]; Cullen Greer[1]; Brian H. Clowers[1]; *[1]Washington 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 Littlejohn[1]; Meng Li[2]; Christopher A. Wootton[2, 3]; Peter B. O'Connor[2]; *[1]University of Warwick, Coventry,, United Kingdom; [2]University of Warwick, Coventry, United Kingdom; [3]Bruker 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]; *[1]State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, China; [2]Department 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 Carlo[1]; Amanda Patrick[1]; *[1]Mississippi 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. Hollerbach[1]; Yehia M. Ibrahim[1]; Vanessa M. Meras[1]; Randolph V. Norheim[1]; Adam P. Huntley[1]; Gordon Anderson[2]; Thomas O. Metz[1]; Robert G. Ewing[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]GAA Custom Electronics, LLC, Benton City, WA*

TP 427 **An interplatform study of three ion mobility techniques to determine lipid collision cross sections**; Anaïs C George[1]; Isabelle Schmitz[1]; Vincent Marie[2]; Benoit Colsch[2]; Florent Rouvière[3]; Sandra Alves[4]; Sabine Heinisch[3]; François Fenaille[2]; Carlos Afonso[1]; Corinne Loutelier-Bourhis[1]; *[1]Laboratoire COBRA, UMR 6014, Université de Rouen, INSA de Rouen, CNRS, IRCOF, Mont Saint Aignan, France; [2]Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), MetaboHUB, F-91191 Gif sur Yvette, France; [3]Université de Lyon, Institut des Sciences Analytiques, UMR 5280 CNRS, 5 rue de la Doua, 69100 Villeurbanne, France; [4]Sorbonne 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 Hynds[1]; Jana M Carpenter[1]; Kelly M Hines[1]; *[1]University of Georgia, Athens, GA*

TP 429 **Development of a high-resolution U-shaped mobility analyzer (UMA) and its applications**; Xiaoqiang Zhang[1]; Kuofeng Tseng[1]; Kang Guo[1]; Yangyue Miao[1]; Lin Liu[1]; Xinfeng Zhou[1]; Wenjian Sun[1]; *[1]Shimadzu Research Laboratory, Shanghai, China*

TP 430 **TW-SLIM Separations Using Asymmetric Radio-Frequency Trapping Fields**; Cullen Greer[1]; Zackary R. Kinlein[1]; Brian H. Clowers[1]; *[1]Washington 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 Muller[1]; Georges Scholl[1]; Johann Far[1]; Edwin De Pauw[1]; Gauthier Eppe[1]; *[1]University of Liège, Liège, Belgium*

TP 432 **Experimental and theoretical determination of the collision cross sections of phosphoric acid clusters: anions compared to cations**; Hélène Lavanant[1]; Valentina Calabrese[2]; Frédéric Rosu[3]; Valérie Gabelica[4]; Carlos Afonso[1]; *[1]Normandie Univ, UNIROUEN, INSA Rouen, CNRS, COBRA, Rouen, France; [2]University of Lyon, University Claude Bernard 1 of Lyon, Institute of Analytical Sciences, CNRS UMR 5280, Villeurbanne, France; [3]CNRS, UMS 3033, Institut Européen de Chimie et Biologie (IECB), Pessac, France; [4]University 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 McBee[1]; Liulin Deng[1]; Adam Engelson[1]; Zongyuan Chen[1]; Daniel Debord[1]; *[1]MOBILion Systems, Inc, Chadds Ford, PA*

TP 434 **Nonlinear Fourier Transform Sweeps in Conjunction with Reduced-Pressure Ion Mobility Mass Spectrometry**; Nathan W. Buzitis[1]; Elvin R. Cabrera[1]; Brian H. Clowers[1]; *[1]Washington State University, Pullman, WA*

TP 435 **Real-time monitoring of dynamic isomer populations with CI-SLIM IMS-MS**; Sonja Klee[1]; Felipe Lopez-Hilfiker[1]; Matthieu Riva[1, 2]; Sebastian Gerber[1]; Urs Rohner[1]; Stephan Graf[1]; Michael Z. Kamrath[1]; *[1]TOFWERK, Thun, Switzerland; [2]Univ. 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 Guzman[1]; Konstantin Ayzikov[2]; Kyle L. Fort[2]; Martin Rykaer[1]; Jeppe Madsen[1]; Ana Martinez Del Val[1]; Alexander A Makarov[2]; Jesper V. Olsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; [2]Thermo 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 Naylor[1]; Brian H. Clowers[2]; Florian Schlottmann[1]; Nic Solle[1]; Stefan Zimmermann[1]; *[1]Leibniz Universität Hannover, Institut für Grundlagen der Elektrotechnik und Messtechnik, Hannover, Germany; [2]Washington State University Department of Chemistry, Pullman, WA*

TP 438 **A new TIMS-MRMS instrument for structural and in-situ analysis of biomolecules**; Anna L Simmonds[1]; Anthony Devlin[2]; Alina Theisen[3]; Gregory Brabeck[3]; Carlos Schat[3]; Christopher A. Wootton[3]; Josephine Bunch[2, 4]; Zoltan Takats[2, 5]; *[1]Rosalind Franklin Institute, Didcot, United Kingdom; [2]Rosalind Franklin Institute, Harwell, Didcot, United Kingdom; [3]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [4]National Physical Laboratory, Teddington, United Kingdom; [5]Imperial 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 Jeon[1]; Carolina Rojas Ramirez[1]; Ruwan T Kurulugama[2]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Agilent 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 Tilmant[1]; Johann Far[1]; Edwin De Pauw[1]; Loic Quinton[1]; *[1]MSLab ULiege, Liege, Belgium*

TP 441 **20 mM Ammonium Carbonate Improves the Detection of Tricarboxylic Acid Cycle Intermediates**; Jarrod A Roach[1]; Laura-Isobel McCall[2]; *[1]University of Oklahoma, Norman, OK; [2]University 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 Chen[1]; Yu-Ching Liu[1]; *[1]China 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 Afjehi[1]; Steffen Waldherr[2]; *[1]University of Vienna/Mass Spectrometry Core Facility- CF SS, Vienna, Austria; [2]University of Vienna/*

Department of Functional and Evolutionary Ecology, Vienna, Austria

TP 444 **IDSL.CSA: MS1 Composite Spectra Analysis to Complement MS2 Annotation in Untargeted Metabolomics Datasets**; Sadjad Fakouri Baygi[1]; Yashwant Kumar[2]; Dinesh Kumar Barupal[1]; *[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 Sun[1]; Yuan Lin[1]; Jeff Op De Beeck[2]; Brandon H. Robson[1]; Joshua A Silveira[3]; Paul Jacobs[2]; Shanhua Lin[1]; *[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 Pellegrinelli[1]; Benjamin Libert[1]; Stephanie Schuster[1]; Conner McHale[1]; *[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 Grasselli[1]; Adriana Arigò[1]; Nicole Marittimo[1]; Giorgio Famiglini[1]; Pierangela Palma[1, 2]; Mansoor Saeed[3]; Simon Perry[3]; Pablo Navarro[3]; Phil Clarke[3]; Mark Brittin[3]; 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 Libert[1]; Barry E Boyes[1]; Chuping Luo[1]; Marc Goldfinger[1]; Mark Haynes[1]; *[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 Beeck[1]; Natalie Van Landuyt[1]; Delphi Van Haver[2, 3]; An Staes[2, 3]; Francis Impens[2, 3]; Xuefei Sun[4]; Yuan Lin[4]; Paul Jacobs[1]; *[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 Urich[1]; Jamie York[1]; John Garrett[2]; Chris Nelson[1]; Justin Steimling[1]; Tim Yosca[1]; *[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 Kim[1]; Sang Beom Han[1]; *[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 Wang[1]; Peng-Kai Liu[2]; Ting-Jia Gu[3]; Bin Wang[3]; Andrew J. Alpert[4]; 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. Leyden[1]; Donald F. Hunt[1, 2]; Jeffrey Shabanowitz[1]; *[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 Aburashed[1]; Thomas Rydzak[1]; Saad Luqman[1]; Ian A Lewis[1]; *[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 Batoon[1]; Lee Bertram[2]; Linfeng Wu[2]; *[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 Fletcher[1]; Jiana Duan[1]; Emily Chea[1]; Robert Egan[1]; Ron Orlando[1, 2]; Scot Weinberger[1]; *[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 Côté[1]; Stephanie Savard[1]; Cynthia Dombrowski[1]; Eugénie-Raphaelle Bérubé[1]; Gabrielle Daigneault[1]; Pierre-Yves Martin[1]; Julie Laquerre[1]; Pascal Mireault[1]; *[1]Laboratoire de sciences judiciaires et de medecine legale, Montreal, QC*

TP 461 **Retention Time Prediction for O-GlcNAc Serine and Threonine Carrying Peptides**; Quinn K Neale[1]; Darien Yeung[1]; Victor Spicer[1]; Helene Perreault[1]; Oleg V. Krokhin[1]; *[1]University of Manitoba, Winnipeg, MB*

TP 462 **Rapid fractionation of human proteome with acidic HILIC Proteome Selective Isolation Chromatography (P-SLICY) for 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 Dattram Pawar[1]; Dr.pramod Kumar[1]; *[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 Elie[1]; Cole Strattman[1]; Jacob Jalali[1]; Jesse Leonard[2]; Erasmus Cudjoe[3]; *[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 Abujrais[1]; Kumari Ubhayasekeraa[1]; Jonas Bergquist[1]; *[1]Uppsala University, uppsala, Sweden*

TP 466 **Analysis of short-chain fatty acids (SCFAs) by LC-MS/MS coupled with chemical derivatization**; Hanpeng Jiang[1]; Zhimin Long[1]; Lihai Guo[1]; *[1]SCIEX, China, Shanghai, China*

TP 467 **Rapid analysis of 11 energy-rich phosphate compounds using the SCIEX Triple Quad 6500+ system**; Junmiao Chen[1]; Dandan Si[1]; Zhimin Long[1]; *[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 Nakatani[1]; Kazuki Ikeda[1]; Masatomo Takahashi[1]; Takeshi Bamba[1]; Yoshihiro Izumi[1]; *[1]Medical Institute of Bioregulation, Fukuoka, Japan*

TP 469 **Targeted analysis of energy metabolites in cells using liquid chromatography-tandem mass spectrometry**; Xiaoyuan Shi[1]; Zhimin Long[1]; Lihai Guo[2]; *[1]SCIEX, China, Shanghai, China; [2]SCIEX, China, Beijing, China*

TP 470 **Determination of Flux into the Tryptophan-Kynurenine Pathway in Biological Samples using Liquid Chromatography Tandem Mass Spectrometry**; Jaeman Byun[1]; Subramaniam Pennathur[1]; Anna Mathew[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 471 **Chiral chromatography in conjunction with LC-MRM-MS for enantiomer-specific resolution of the oxylipidome**; Liping Yang[1]; Jaewoo Choi[2]; Jan F. Stevens[2, 3]; Claudia Maier[1, 2]; *[1]Department of Chemistry, Oregon State University, Corvallis, OR; [2]Linus Pauling Institute, Oregon State University, Corvallis, OR; [3]Department of Pharmaceutical Sciences, Oregon State University, Corvallis, OR*

TP 472 **Multiple Reaction Monitoring (MRM) Method Development for Quantitation of Spermidine in Whole Blood**; Jericha Mill[1]; Cameron Kaminsky[1]; Thomas Raife[2]; Lingjun Li[1, 3]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [2]University of Wisconsin School of Medicine and Public Health, Department of Pathology and Laboratory Medicine, Madison, WI; [3]University of Wisconsin-Madison, School of Pharmacy, Madison, WI*

TP 473 **Measurement of Phthalates using Liquid Chromatography-Mass Spectrometry**; Abu Hena Mostafa Kamal[1]; Vasanta Putluri[2]; Chandra Shekar Reddy Ambati[2]; Bhagavatula Moorthy[2]; Chris Amos[2]; Nagireddy Putluri[2]; *[1]Baylor College of Medicine, Houston, TX; [2]Baylor 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]; *[1]SHIMADZU Corporation, Kyoto, Japan; [2]Osaka 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. Wudy[1]; Verena K. Mittermeier-Kleßinger[1]; Sapna Sharma[1]; Andreas Dunkel[2]; Karin Kleigrewe[3]; Regina Ensenauer[4, 5, 6]; Corinna Dawid[1, 3]; Thomas F. Hofmann[1]; *[1]Chair of Food Chemistry and Molecular Sensory Science, Technical University of Munich, Freising, Germany; [2]Leibniz-Institute for Food Systems Biology at the Technical University of Munich, Freising, Germany; [3]Bavarian Center for Biomolecular Mass Spectrometry, Technical University of Munich, Freising, Germany; [4]Institute for Medical Information Processing, Biometry, and Epidemiology (IBE), Ludwig-Maximilians-Universität München, Munich, Germany; [5]Division of Pediatric Cardiology and Intensive Care, University Hospital, Ludwig-Maximilians-Universität München, Munich, Germany; [6]Institute 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 Conway[1]; Jan-Christoph Wolf[2]; Christoph Haisch[3]; *[1]UNC Charlotte, CHARLOTTE, NC; [2]Plasmion GmbH, Augsburg, Germany; [3]Technical 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 Moritz[3]; *[1]Department of Forest Genetics and Plant Physiology, Swedish University of Agricultural Sciences, Umeå, Sweden; [2]Swedish Metabolomics Centre, Umeå, Sweden; [3]Novo 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 Annangudi[1]; Scott Greenwalt[1]; Jeffrey Simpson[1]; *[1]Corteva Agriscience, Indianapolis, IN*

TP 479 **Reliable quantification of adenylate nucleotides using ultra-performance liquid chromatography-tandem mass spectrometry (UPLC-MS/MS)**; Maleesha De Silva[1]; Kyle Fulghum[1]; David Hoetker[1]; Bradford G Hill[1]; Pawel K Lorkiewicz[1]; *[1]University 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. Engevik[3]; Amy Engevik[3]; *[1]Baylor College of Medicine, Houston, Texas; [2]Texas Children's Hospital, Dept. of Pathology, Houston, Texas; [3]Medical University of South Carolina, Charleston, SC*

TP 481 **Analysis of Polyamine Metabolism by Liquid Chromatography-High Resolution Mass Spectrometry**; Bao Tran[1]; Lin Tan[2]; Thomas D Horvath[3]; Sara A Martinez[1]; John Weinstein[1]; Philip Lorenzi[1]; *[1]University of Texas MD Anderson Cancer Center, Houston, TX; [2]MD Anderson Cancer Center, Houston, TX; [3]Baylor College of Medicine, Houston, Texas*

TP 482 **Targeted metabolite analysis of polyamine synthesis and metabolism by LC-MRM/MS**; Katelyn G. McMurray[1]; Jun Han[1, 2]; Juncong Yang[1]; Molly McCormack[1]; Gillian Leach[1]; Kiara Kumar[1]; Dave Schibli[1, 2]; David R. Goodlett[1, 3]; *[1]Genome BC Proteomics Centre, University of Victoria, Victoria, BC; [2]Division of Medical Sciences, University of Victoria, Victoria, BC; [3]Department 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 Yang[1]; Molly McCormack[1]; Kiara Kumar[1]; Katelyn G. McMurray[1]; Gillian Leach[1]; Dave Schibli[1, 2]; David R. Goodlett[1, 3]; *[1]Genome BC Proteomics Centre, University of Victoria, Victoria, BC; [2]Division of Medical Sciences, University of Victoria, Victoria, BC; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC*

TP 484 **A High-Efficiency Method for simultaneous Quantification of Seven Classes of Phytohormones**; Lingyun Chen[1]; Yun Zhao[1]; Qidan Li[1]; Jin Zi[1]; *[1]BGI-Shenzhen, Shenzhen, China*

TP 485 **Targeted metabolic analysis of bile acids in biological samples by ultra-performance liquid chromatography tandem mass spectrometry**; Yun Zhao[1]; Yang Feng[1]; Hongkai Xu[1]; Qidan Li[1]; Jin Zi[1]; *[1]BGI-Shenzhen, Shenzhen, China*

TP 486 **LOD and LOQ determination of metabolites by using OT2 liquid handler and HILIC/PFPP columns on a OrbitrapTMID-XTMMass Spectrometer**; Didar Asik[1]; Vyncent Nguyen[1]; Sarah Baron[1]; Chengjian Tu[1]; *[1]Thermo 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 Nguyen[1]; Chengjian Tu[1]; *[1]Thermo 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. Bolte[3]; Thomas D Horvath[1, 2]; Maxim Daniel Seferovic[3]; Kathleen M. Hoch[1, 2]; Derek Steven O'Neil[3]; James Versalovic[1, 2]; Anthony Haag[1, 2]; Kjersti Aagaard[3]; *[1]Texas Children's Hospital - Microbiome Center, Houston, TX; [2]Baylor College of Medicine, Houston, Texas; [3]Department 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

Guo[1]; Adi Kulkarni[2]; Danielle Moore[2]; Kate Yu[2]; *[1]Avice Labs, Acton, MA; [2]908 Devices, Boston, MA*

TP 490 **Comparing Targeted LC-MS/MS and Untargeted GC-MS for the analysis of Kynurenine Pathway in Plasma Samples**; Luis M Valdiviez[1]; Uri Keshet[1]; Oliver Fiehn[1]; *[1]West Coast Metabolomics Center, Davis, CA*

TP 491 **Quantitative analysis of antimicrobial compounds from Pseudomonas protegens**; Samantha J Balboa[1]; Shilu Dahal[2]; Clemencia M. Rojas[2]; Leslie M. Hicks[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]University of Nebraska-Lincoln, Lincoln, NE*

TP 492 **Quantitative Analysis of Polar Metabolites with Comprehensive Plasma and Cell Targeted Metabolomics Workflow**; Karen E Yannell[1]; Cate Simmermaker[1]; Genevieve C Van de Bittner[1]; *[1]Agilent 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 Campbell[1]; Timothy Kassis[1]; Sofia Costa[1]; Jeff Pruyne[1]; Luke Ferro[1]; Joshua D Lauterbach[1]; Steven Hooper[1]; Jack Howland[1]; Gabriel Asher[1]; Mimoun Cadosch Delmar[1]; J. M. Geremia[1]; *[1]Matterworks, 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 Groves[1]; Thomas Rydzak[1]; Raied Aburashed[1]; Stephanie L Bishop[1]; Maryam Mapar[1]; Carly C Y Chan[1]; Ian A Lewis[1]; *[1]University of Calgary, Calgary, AB*

TP 495 **Absolute quantification of cellular metabolites in bioprocessing samples using machine learning**; Luke S Ferro[1]; Jack Howland[1]; Timothy Kassis[1]; Ana S.H. Costa[1]; Jeff Pruyne[1]; Steven Hooper[1]; Joshua D Lauterbach[1]; Gabriel Asher[1]; Mimoun Cadosch Delmar[1]; J. M. Geremia[1]; Jennifer M Campbell[1]; *[1]Matterworks, Somerville, MA*

TP 496 **High-Throughput Scheduled Parallel Reaction Monitoring Mass Spectrometry of Tryptophan-Indole Metabolites in Culture Supernatant of Human Bacterial Isolates**; Huidi Tian[1]; Elizabeth Fleming[2]; Lina Kozhaya[2]; Rachel Hardy[2]; Derya Unutmaz[2]; Julia Oh[2]; Xudong Yao[1]; *[1]University of Connecticut, Storrs, CT; [2]The 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 Alam[1]; Armando Alcazar Magana[1]; Jaewoo Choi[1]; Luke Marney[1]; Paul Cheong[1]; Mikah Brandes[2]; Cody Neff[2]; Amala Soumyanath[2]; Jan F. Stevens[1]; Claudia Maier[1]; *[1]Oregon State University, Corvallis, OR; [2]Oregon Health & Science University, Portland, Oregon*

TP 498 **Analysis for Erinacines and Hericenones in Lion’s Mane Mushrooms using HRMS and Ion Mobility**; Gordon T. Fujimoto[1]; Sarah E. Dowd[1]; Lindsay E. Hatch[1]; Emily R. Britton[1]; *[1]Waters 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. Inutan[1]; Kathleen C. Aligaya[1]; Asia Catherine M. Mahayag[1]; Johayber Sarip[1]; Enjelyn C. Gomez[1]; Sarah Trimpin[2]; Charles N. McEwen[3]; *[1]Mindanao State University-Iligan Institute of Technology, Iligan City, Philippines; [2]Wayne State University, Detroit , MI; [3]Research 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 Deng[1]; Jennifer L Kolwich[1]; Haidy Metwally[1]; Avena C Ross[1]; Richard D Oleschuk[1]; *[1]Queen's University, Kingston, ON*

TP 501 **Characterization of Conus textile crude venom by capillary electrophoresis hyphenated to mass spectrometry**; Fabrice Saintmont[1]; Yoann Ladner[1]; Sébastien Dutertre[1]; Claudia Bich[1]; *[1]Univ. 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. Thomas[5]; Lloyd W. Sumner[1, 2, 3, 4]; *[1]Department of Biochemistry, University of Missouri-Columbia, Columbia, MO; [2]Metabolomics Center, University of Missouri-Columbia, Columbia, MO; [3]Interdisciplinary Plant Group, University of Missouri-Columbia, Columbia, MO; [4]Christopher S. Bond Life Sciences Center, University of Missouri-Columbia, Columbia, MO; [5]Southwest 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 Perera[1]; Bonnie Rogers[1]; Andrew L. Thomas[1]; Michael Greenlief[1]; *[1]University of Missouri-Columbia, Columbia, MO*

TP 504 **Therapeutic applications of semi-synthetic analogs derived from newly discovered variants of the antifungal occidiofungin**; Nopakorn Hansanant[1]; Ravi Orugunty[2]; James Leif Smith[1, 2]; *[1]Texas A&M University, College Station, TX; [2]Sano Chemicals, Bryan, TX*

TP 505 **Application of molecular network in the differentiation of metabolic profiles of actinobacteria**; Talita Carla de Tralia Medeiros[1]; Luiz Alberto Beraldo De Moraes[1]; *[1]Universidade de São Paulo, Ribeirão Preto, Brazil*

TP 506 **Biophysical characterisation of DNA triplexes for antigene technology**; Jack Klose[1]; Alexander Begbie[1]; Tara L Pukala[1]; *[1]University of Adelaide, Adelaide, Australia*

TP 507 **Determination of molecular weight of small interfering nucleotides siRNA by LCMS**; Jia Zheng[1]; Xia Qiao Liu[1]; Yuan Hong Hao[1]; Hong Tao Huang[1]; *[1]Shimadzu(China)Co.,LTd, Shanghai, China*

TP 508 **Information-rich spectral libraries from nucleobases and deoxynucleosides facilitate the identification of ribonucleosides by nLC-MSMS**; Guadalupe Espadas[1]; Eduard Sabidó[1]; *[1]Proteomics Unit, Center for Genomic Regulation, Universitat Pompeu Fabra, Barcelona, Spain*

TP 509 **Flavonoid Derivatives: A Novel Triplex-Binding Ligand**; Landy Gu[1]; Vanessa M. Rangel[1]; Nghia Tran[1]; Douglas Chu[1]; Liang Xue[1]; *[1]University of the Pacific, Stockton, CA*

TP 510 **Human RNase 4 improves mRNA sequence characterization by LC–MS/MS**; Eric Wolf[1]; Sebastian Grünberg[1]; S. Hong Chan[1]; Nan Dai[1]; Tien-Hao Chen[1]; Erbay Yigit[1]; Ivan R Correa Jr. [1]; *[1]New England Biolabs, Inc., Beverly, MA*

TP 511 **Accelerating Oligonucleotide Research Using Novel Bioinert LC, QTOF and TQ LC-MS**; Mridul Mandal[1]; Brian Domanski[1]; Xiaomeng Xia[1]; Nivesh Mittal[1]; *[1]Shimadzu Scientific Instrument, Columbia, Maryland*

TP 512 **tRNAs and tRNA modifications correlated to metastasis in melanoma via LC-MS and tRNA-seq analysis**; Cassandra Herbert[1]; Balasubrahmanyam Addepalli[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 513 **In-Source CID of Modified Oligonucleotides Analyzed by IP-RP LCMS: Effects of Experimental Parameters**; Stilianos G. Roussis[1]; Claus Rentel[1]; *[1]Ionis Pharmaceuticals, Inc., Carlsbad, CA*

TP 514 **Molecular weight confirmation and impurity analysis of a 70-mer oligonucleotide**; Remco Van Soest[1]; Sahana Mollah[2]; Kerstin Pohl[3]; Ling Huang[4]; *[1]SCIEX, Redwood City, CA; [2]Sciex, Redwood City, CA; [3]Sciex, Framingham, MA; [4]Integrated DNA Technologies, Coralville, IA*

TP 515 **OligoDistiller: An MS-platform agnostic software tool developed particularly for MS data analysis of complex**

oligonucleotide samples and their impurities; Youzhong Liu[1]; Piotr Prostko[2]; Dirk Valkenborg[2]; Jennifer L Lippens[1]; Ronald De Vries[1]; Thomas De Vijlder[1]; *[1]Janssen Pharmaceutica NV, Beerse, Belgium; [2]Hasselt University, Hasselt, Belgium*

TP 516 **Competitive Transcription and Adduct Bypass Assay for Examining Transcriptional Perturbations and Repair of O2-Alkylthymidine Lesions**; Chen Wang[1]; Xiaomei He[1]; Yinan Wang[1]; Yinsheng Wang[1]; *[1]UCR, Riverside, CA*

TP 517 **Direct chemical characterization of double-stranded oligonucleotides crosslinked by the microbiome-derived genotoxin colibactin by high-resolution mass spectrometry**; Chiara Lecchi[1]; Erik S. Carlson[2]; Peter W. Villalta[1]; Emily P. Balskus[2]; Silvia Balbo[1, 3]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, MN; [2]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA; [3]School of Public Health, University of Minnesota, Minneapolis, MN*

TP 518 **Microflow liquid chromatography – nanoelectrospray mass spectrometry of oligonucleotides**; Guilherme Jendiroba Guimaraes[1]; Franklin E Leach III[1]; Michael G Bartlett[1]; *[1]University of Georgia, Athens, GA*

TP 519 **Tandem mass spectrometry quantification of Oligonucleotides using an isobaric internal standard**; Christopher Gawlig[1]; Güngör Hanci[1]; Michael Ruehl[1]; *[1]BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany*

TP 520 **Localization of phosphorothioate linkages in partially phosphorothioated oligonucleotides**; Samuel P Wein[1]; Trenton M Peters-Clarke[2]; Oliver Kohlbacher[3]; *[1]University of Tübingen, Tübingen, Germany; [2]University of Wisconsin, Madison, WI; [3]University 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 Uchiyama[1]; Yoshihiro Kunimura[1]; Simon Ashton[2]; Richard Price[2]; Helen Jose[2]; Atsuhiko Toyama[1]; Neil Loftus[2]; *[1]SHIMADZU Corporation, Kyoto, Japan; [2]Shimadzu, 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 Raemdonck[1]; Kristina Wicht[1]; Jessika Wynendaele[1]; Eddy Ruijter[1]; Koen Iterbeke[1]; *[1]AnaBioTec, 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 Kenderdine[1]; Daniele Rollo[1]; Daniele Fabris[1, 2]; *[1]University of Connecticut, Storrs, CT; [2]RiboDynamics LLC, Manchester, Connecticut*

TP 524 **Extending the Concept of Spectral Accuracy to the Deconvolution of Multiply Charged Large Molecules**; Yongdong Wang[1]; Stacey Simonoff[1]; Don Kuehl[1]; Nan Zhang[2]; Qingfei Zheng[2]; *[1]Cerno Bioscience, Las Vegas, NV; [2]Department of Radiation Oncology, College of Medicine, Columbus, Ohio 43210*

TP 525 **Characterization of Nucleic Acid Fragment Ions by Isotopic Distributions**; Michael B Lanzillotti[1]; Jessica G Pauling[1]; Jennifer S Brodbelt[1]; *[1]University 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 Slobodchikova[1]; Wei Lu[1]; *[1]Alliance 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 Tran[1]; Steven Fletcher[1]; Jace W Jones[1]; *[1]University 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 Szot[1]; Kristina Hakansson[2]; *[1]University of Michigan, Ann Arbor, MI; [2]University 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 Kato[1]; Kosuke Uchiyama[1]; Hiroyuki Yasuda[1]; Simon Ashton[2]; Richard Price[2]; Helen Jose[2]; Neil Loftus[2]; Kiyoshi Kakiya[3]; Atsuhiko Toyama[1]; *[1]SHIMADZU Corporation, Kyoto, Japan; [2]Shimadzu Corporation, Manchester, United Kingdom; [3]Peptistar Inc., Settsu, Japan*

TP 530 **Optimized Fragmentation of Oligonucleotides Suppresses Undesired Fragmentation Products and Enables Confident Sequence Assignment**; Joshua Hinkle[1]; William M. McGee[2]; Joshua P. Salem[3]; Robert L Ross[4]; Christopher Mullen[1]; Scott Kronewitter[2]; John E.P. Syka[1]; James L. Stephenson[2]; *[1]Thermo Fisher Scientific, San Jose, California; [2]Thermo Fisher Scientific, Lexington, Massachusetts; [3]University of Michigan Ann-Arbor, Ann Arbor, MI; [4]Thermo 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]; *[1]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; [2]Center for RNA Biology, The Ohio State University, Columbus, OH; [3]Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; [4]The 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 Rollo[1]; Adi Kulkarni[2]; Kate Yu[2]; Hampus Engstroem[2]; Guillaume Tremintin[3]; Daniele Fabris[1]; *[1]University of Connecticut, Storrs, CT; [2]908 Devices, Boston, MA; [3]Bruker 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 Matsubara[1]; Yasuto Yokoi[1]; Jonathan Fox[2]; Maissa Gaye[3]; Joe Fredette[3]; Matthew A Lauber[3]; Guillaume Bechade[2]; Masami Koike[4]; Yuko Nobe[5]; Masato Taoka[5]; Hiroshi Nakayama[4]; *[1]Mitsui knowledge, Minato, Japan; [2]Waters S.A.S, Saint-Quentin, France; [3]Waters Corporation, milford, MA; [4]RIKEN Center for Sustainable Resource Science, Wako, Japan; [5]Tokyo Metropolitan University, Hachioji, Japan*

TP 534 **Metabolite Profiling and Identification of Oligonucleotide in In Vitro Metabolic System**; Gengyao Qin[1]; Qiandan Miao[1]; Liqi Shi[1]; Zhiyu Li[1]; Weiqun Cao[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi 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 Heel[1]; Kathrin Breuker[2]; *[1]Institute of Organic Chemistry and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, Austria; [2]Institute 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 Hackbusch[1]; Gary Held[2]; Kenton Chodara[2]; Syed K Raza[2]; Yi Zhang[1]; Min Du[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Milwaukee, WI; [3]Thermo Fisher Scientific, Franklin, MA*

TP 537 **Fractionation of complex RNA mixtures for LC-MS/MS**; Jennifer Kist[1]; Cassandra Herbert[1]; Patrick Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

TP 538 **High-Resolution Accurate Mass Orbitrap mRNA Analysis: Poly-A Tail, Capping Analysis, and Bottom-up Sequence Mapping**; Alice Guo[1]; Kevin Kun Guo[1]; *[1]Avice Laboratories, Acton, Massachusetts*

TP 539 **A method for predicting the monoisotopic mass in high-resolution mass spectra of oligonucleotides**; Piotr Prostko[1]; Youzhong Liu[2]; Thomas De Vijlder[2]; Tatsiana Khamiakova[2]; Dirk Valkenborg[1]; *[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 Knowles[1]; Jo-Anne Riley[2]; Jonathan Fox[2]; Catalin E Doneanu[3]; Ying Qing Yu[3]; *[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 Nakayama[1]; Masami Koike[1]; Yuko Nobe[2]; Masato Taoka[2]; *[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 Pandey[1]; Adarsh K Mayank[2]; James A Wohlschlegel[2]; *[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 Wilhelm[3]; 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 Xu[1]; Ling Ling[1]; Chuan-Fan Ding[1]; Liang Wang[2]; Kate Yu[3]; *[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 Quantifya NovelBispecific Peptide by SPE–UPLC-MS/MS in Human Plasma Tre**; Andy (hongfang) Xue[1]; Pengliang Ren[2]; Yu Yang[1]; Ruiling Wang[2]; Aihua Liu[1]; *[1]Alliance Pharma, Malvern, PA; [2]Shaanxi Micot Technology, Xi'xian New Area, China*

TP 546 **Integrated calibration curve-based absolute quantification of samples in SpectroDive**; Veronique Laforte[1]; Maik Müller[1]; Magdalena Domitrz[1]; Tejas Gandhi[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

TP 547 **A Robust Protein Normalization Strategy for Comparing Protein Expression Levels Across Tissues and Species by PRM**; Joshua Nicklay[1]; Jingjing Deng[1]; Eugene Ciccimaro[1]; Petia Shipkova[1]; *[1]Bristol-Myers Squibb, Princeton, NJ*

TP 548 **The Proteomes that Feed the World**; Gian Luca Corongiu[1]; Sarah Brajkovic[1]; Patrick Roehrl[1]; Andrea Piller[1]; Sebastian Urzinger[1]; Lukas Wuerstl[1]; Paula Andrade Galan[1]; Guido Giordano[1]; Veronica Ramirez[1]; Ezgi Aydin[1]; Genc Haljiti[1]; Mario Picciani[1]; Qussai Abbas[1]; Cemil Can Saylan[1]; Armin Soleymaniniya[1]; Jiuyue Pan[1]; Sophia Hein[1]; Corinna Dawid[1]; Stephanie Heinzlmeir[1]; Claus Schwechheimer[1]; Chris Schoen[1]; Viktoriya Avramova[1]; Josch Pauling[1]; Christina Ludwig[1]; Dmitrij Frishman[1]; Mathias Wilhelm[1]; Caroline Gutjahr[1]; Ralph Hueckelhoven[1]; Brigitte Poppenberger[1]; Bernhard Kuster[1]; *[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**; Aiying Yu[1]; Lingyao Meng[1]; Jintang He[1]; Surinder Kaur[1]; Keyang Xu[1]; *[1]Genentech Inc., South San Francisco, CA*

TP 550 **Building high-throughput analytical methods for monitoring peptide biomarkers in equine athletes**; Cecily R Wood[1]; Abigail Burrows Franco[1]; Alison Porter[1]; Scott M Peterman[2]; Scott D Stanley[1]; *[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 Gao[1]; Na Li[1]; Yanfu Ren[1]; Zhiyu Li[2]; Lili Xing[2]; Yi Tao[2]; Liang Shen[2]; *[1]WuXi AppTec, Suzhou, China; [2]WuXi AppTec, Shanghai, China*

TP 552 **Optimizing lower limits of quantification and detection by choosing transitions in Skyline**; Nicholas Shulman[1]; Lilian Heil[1]; Philip M Remes[2]; Michael J. MacCoss[1]; *[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 Romanova[1]; David C Platt[2, 3]; Joseph M. Williams[4]; David L. Cedeño[3, 4]; Ricardo Vallejo[3, 4]; Jonathan V. Sweedler[5]; *[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. Turmon[1]; Andrew Palmer[1]; Alexander W. Sun[1]; Lisa Boatner[1]; Keriann M. Backus[1]; *[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 Ritz[1]; Christian Schori[1]; Emmanuelle Lezan[2]; Alexander Schmidt[1]; *[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 Lehe[1]; Erin Jeffery[1]; Abdullah Abood[1]; Charles Farber[1]; Gloria Sheynkman[1]; *[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. Martinez[1]; Eric Kuhn[1]; Susanne B. Breitkopf[1]; Yogesh Chutake[1]; Jessica Filiatrault[1]; Min Yuan[1]; Yatao Shi[1]; Dirk M. Walther[1]; Dapeng Chen[1]; Brad Enerson[1]; Stefanie Schalm[1]; Joyoti Dey[1]; Alice McDonald[1]; Matt Weiss[1]; Juliet Williams[1]; Chris De Savi[1]; Kirti Sharma[1]; *[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'Meally[1]; Peter M. Abadir[1]; Robert N. Cole[1]; Brian Foster[1]; *[1]Johns Hopkins School of Medicine, Baltimore, MD*

TP 559 **Quality profiling of Tetracosactide injections using HPLC-HRMS**; Janez Ilaš[1]; Aleksandra Bračko[2]; *[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 Menyhart[1]; Laszlo Gyenis[1]; Kristina Jurcic[1]; David W Litchfield[1]; *[1]University of Western Ontario, London, ON*

TP 561 **Ocular tissue distribution and systemic pharmacokinetics of a biotherapeutic protein**; Emily Werth[1]; Lin-Zhi Chen[1]; *[1]Boehringer Ingelheim, Ridgefield, CT*

TP 562 **A novel approach for generation of retention time - molecular mass chromatograms for improving**

interpretation and quantification of biotherapeutic molecules; Martin Green[1]; Keith Richardson[1]; Mark Wrona[2]; Yun Alelyunas[2]; Steve Bajic[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters 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 Maheshwari[1]; Robert Popp[1]; Christoph H. Borchers[2, 3, 4, 5]; *[1]MRM Proteomics Inc., Montréal, QC; [2]Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [3]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [4]Division of Experimental Medicine, McGill University, Montreal, QC; [5]Department 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 Feng[1]; Daniel Wall[1]; Jennifer Cunliffe[1]; Manisha Saxena[2]; Charlie G. Knutson[1]; Robert Dodge[3]; Elena Fernandez[4]; *[1]Novartis Institutes for Biomed.Research, Inc., Cambridge, MA; [2]Novartis Pharma AG, Basel, Switzerland; [3]Novartis Pharmaceuticals, East hanover, New Jersey; [4]Molecular 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 Alba[4]; Sarah Cianferani[4]; Rabah Gahoual[2]; Yannis Nicolas Francois[5]; *[1]Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, France; [2]Unité de Technologies Chimiques et Biologiques pour la Santé (UTCBS), CNRS UMR8258, Inserm U1022, Université de Paris, France; [3]Laboratoire de Toxicologie Biologique, Hôpital Lariboisière, Assistance Publique – Hôpitaux de Paris (AP-HP), France; [4]Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO) IPHC UMR 7178, Université de Strasbourg, France; [5]Laboratoire 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 Heusel[1]; Stephen Lock[2]; Nick Morrice[2]; Sibylle Heidelberger[2]; Jakob Bunkenborg[1]; Michael Barrett Andersen[1]; Nicolai Bache[1]; *[1]Evosep Biosystems, Odense, Denmark; [2]SCIEX, Macclesfield, United Kingdom*

TP 567 **Advances in Intact Protein Quantitation using Gábor Transform-Based Tools in iFAMS**; Kayd L. Meldrum[1]; Andrew K. Swansiger[1]; Meghan M. Daniels[1]; Crystal Kirmiz Cody[2]; Wendi A. Hale[2]; David L. Wong[2]; Michael D. Knierman[2]; Xi Qiu[2]; John Sausen[2]; James S. Prell[1, 3]; *[1]University of Oregon, Department of Chemistry and Biochemistry, Eugene, OR; [2]Agilent Technologies, Inc., Santa Clara, CA; [3]Materials Science Institute, University of Oregon, Eugene, OR*

TP 568 **Development of Quantitative cGMP Impurity Protein Assays Supporting Diverse Modalities, Part II: Analysis**; Chelsea M Desbiens[1]; Gustavo H M F Souza[1]; Michael J Nold[1]; *[1]KBI Biopharma, Durham, NC*

TP 569 **Development of Quantitative cGMP Impurity Protein Assays Supporting Diverse Modalities, Part I: Discovery**; Gustavo H M F Souza[1]; Chelsea M Desbiens[1]; Michael J Nold[1]; *[1]KBI 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 Gorre[1]; Lauren M Kraft[2]; Chris Sauer[2]; Alexander N Barnakov[2]; Andrew Mahan[2]; Thomas Kelly[2]; Hirsh Nanda[2]; Partha Chowdhury[2]; *[1]Janssen Research and Development, Spring House, PA; [2]Johnson & Johnson, Spring House, PA*

TP 571 **New USP Standards and Tools to Support Mass Spectrometry Based Multi-Attribute Method (MAM) for Therapeutics Proteins**; Li Jing[1]; Jingzhong Guo[1]; Kevin Carrick[1]; Diane McCarthy[1]; *[1]USP, 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 Bannwart[1]; Neelanjan Bose[1]; *[1]Emery Pharma, Alameda, CA*

TP 573 **Multiplex quantitation of critical host cell proteins(HCPs) using a SureQuant mass spectrometry assay peptide panel**; Jae Choi[1]; Bhavin Patel[1]; Terry Hicks[2]; Matthew Daniels[2]; Sarah Baron[3]; Km Shams Ud Doha[3]; Paul Gulde[3]; Scott M Peterman[4]; Nikki Jarrett[1]; Kay Opperman[1]; Ryan Bomgarden[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, St Louis, MO; [3]Thermo Fisher Scientific, Grand Island, NY; [4]Thermo 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-Rangel[1]; Zeshan G Aqeel[1]; *[1]Phenomenex, Torrance, CA*

TP 575 **Automated Data Analysis Workflow Leveraging PASEF Data Accelerates Confident Detection of Low-Abundance HCPs**; Amy Claydon[1]; Guillaume Tremintin[2]; Juergen Kastler[3]; Stuart Pengelley[4]; Jonathan Krieger[2]; Arnd Brandenburg[3]; *[1]Genedata Ltd, Cambridge, United Kingdom; [2]Bruker, San Jose, CA; [3]Genedata AG, Basel, Switzerland; [4]Bruker 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 Yu[1]; Kellen Delaney[1]; Samantha Ippoliti[1]; Robert E. Birdsall[1]; *[1]Waters 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 Okrasa[1]; Jana Broecker[1]; Anna Cooper[1]; Aneta Dębicka[1]; Maria Serrano-Vega[1]; Nicolae Solcan[1]; Stacey Southall[1]; *[1]Sosei 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 Prevost[3]; Nathalie Barilone[3]; Korantin Le Mouël[4]; Manuela Zoonens[4]; Pierre-Jean Corringer[3]; Sarah Cianferani[1, 2]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO), Université de Strasbourg, CNRS, IPHC, UMR 7178, Strasbourg, France; [2]Infrastructure Nationale de Protéomique ProFI, FR2048 CNRS CEA, Strasbourg, France; [3]Channel-Receptors Unit, Institut Pasteur, CNRS, UMR 3571, Paris, France; [4]Laboratoire 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 Wang[1]; Peter K Lundquist[2]; Liangliang Sun[1]; *[1]Michigan State university, EAST LANSING; [2]Michigan 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]; *[1]Nanobiology Institute, Yale University, West Haven, Connecticut; [2]Department of Cell Biology, Yale University School of Medicine, New Haven, Connecticut*

TP 581 **Analysis of lipid transport mechanisms via native mass spectrometry**; Tobias Rath[1]; Rene Zangl[1]; Nils Hellwig[1];

Nina Morgner[1]; [1]*Goethe-University, Insitute of Physical and Theoretical Chemistry, Frankfurt am Main, Germany*

TP 582 **Deciphering multi drug resistance protein1 lipid trafficking using native mass spectrometry top-down approach**; Maya Miller[1]; Tarick El-Baba[1]; Carol V Robinson[1]; [1]*Oxford Univerisity, 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 Hinkle[3]; Christopher Mullen[3]; John E.P. Syka[3]; 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 Rödström[4]; 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 Jung[1]; Kyowon Jeong[3]; Jared Shaw[4]; Moitrayee Bhattacharyya[2]; Kallol Gupta[1]; [1]*Yale School of Medicine, Department of Cell Biology, New Haven, CT;* [2]*Yale School of Medicine, Department of Pharmacology, New Haven, CT;* [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 Robinson[1]; Carmen Fernandez-Metzler[2]; Serge Zemerov[2]; Richard King[2]; Tanvi Desai[1]; Michael Lyman[1]; Jessica Peters[1]; Christopher Gibson[1]; Weixun Wang[1]; [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 Hinkle[3]; Idlir Liko[4]; Jack L Bennett[1, 2]; Andrew Dolan[1, 2]; Christopher Mullen[3]; John E.P. Syka[3]; 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 Lima[1]; Maggy Lepine[1]; Lekha Sleno[1]; [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 Wu[1]; Jea Park[1]; Gennifer Merrihew[1]; Kristine Tsantilas[1]; Ireshyn Govender[2]; Sindisiwe Buthelezi[3]; Justin Jordaan[2]; Stoyan Stoychev[2]; Michael J. MacCoss[1]; [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 Lacey[1]; Marius M. Kostelic[1]; 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-Jacques[1]; Kyung-No Son[2]; Dhara Shah[1]; Sang Min Lee[2]; Vinay Kumar Aakalu[2]; Stephanie M Cologna[1]; [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 Jheng[1]; San-Yuan Wang[2]; Ya-Hsuan Chang[3]; Hsuan-Yu Chen[3]; Chia-Li Han[2]; [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 Ashima[1]; Han Le[1]; Saiful Chowdhury[1]; [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 Nields[1]; Scott Mack[2]; Robert Hepler[3]; Andrew Mahan[3]; Chelsea Leonce[3]; Mariam Elnaggar[2]; Maggie Ostrowski[2]; Hirsh Nanda[3]; [1]*Janssen Biopharmaceticals, 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. Young[1]; Karl F. Poncha[1]; 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. coliStrains with a Reduced Repertoire of Anti-Oxidation Defense Enzymes by Mass Spectrometry**; Yanjia Zhang[1]; Sanjay Kumar Rohaun[2]; James A. Imlay[2]; Aaron Timperman[1]; [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. Maity[1]; Jerry C. Dinan[1]; Stewart R. Durell[1]; Andrew J. Perciaccante[1]; Daniel H. Appella[2]; Lisa M. Jenkins[1]; [1]*Laboratory of Cell Biology, Center for Cancer Research, National Cancer Institute, Bethesda, MD;* [2]*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 Spectrometric Approaches**; Emily K Wright[1]; Michael Hayes[1]; James Pesavento[1]; [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 Day[1]; Xiaolu Li[1]; Matthew J Gaffrey[1]; James Sanford[1]; Tyler Sagendorf[1]; Kwame Attah[1]; Sue Bodine[2]; Joshua Adkins[1]; Weijun Qian[1]; [1]*Pacific*

Northwest National Laboratory, Richland, WA; [2]Oklahoma Medical Research Foundation, Oklahoma City, OK

TP 601 **Optimization of a diaPASEF method for phosphoproteomics analysis of mouse brain tissues**; Marie Gebelin[1]; Christine Schaeffer[1]; Jeewan Babu Rijal[1]; Christine Carapito[1]; [1]*Laboratoire 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 Liu[1]; Sagar Kathuria[1]; Joel Bucci[1]; Kyle Cole[1]; Pierrick Rival[2]; Bailin Zhang[1]; Alessandro Masiero[2]; [1]*Sanofi, Cambridge, MA; [2]Sanofi, Vitry-sur-Seine, France*

TP 603 **Investigating the post-translational regulation of tardigrade cryptobiosis**; Evan R. Stair[1]; Abel A. Salas[1]; Leslie M. Hicks[1]; [1]*University 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 Forrester[1]; Aleksandra Tata[1]; Purushothama Rao Tata[1]; Matthew W Foster[1]; [1]*Duke 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 Liu[1]; Roxana McCloskey[1]; Zoe Zhang[1]; [1]*SCIEX, Framingham, MA*

TP 606 **A novel role for ERp46 in platelet function revealed by IodoTMT & LC-MS/MS/MS**; Junsong Zhou[1]; Tong Liu[2]; Yi Wu[3]; Hong Li[2]; David W. Essex[3]; [1]*Columbia University, New York, NY; [2]Rutgers New Jersey Medical School, Newark, NJ; [3]Sol Sherry Thrombosis Research Center, Temple University School of Medicine, Philadelphia, PA*

TP 607 **Identification of glycated peptides using similarity of MS/MS spectrum**; Hyejin Kim[1]; Heeyoun Hwang[2]; Insung Yong[1]; Pilnam Kim[1]; Jin Young Kim[2]; [1]*Department of Bio and Brain Engineering, KAIST, Daejeon, South Korea; [2]Korea 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 Gaffrey[2]; Xiaolu Li[2]; Bin Yang[1]; Wei-Jun Qian[2]; Tong Zhang[2]; [1]*Department of Biological Systems Engineering, Washington State University, Richland, WA; [2]Biological 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]; [1]*Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; [2]Graduate 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 Cornelius[1]; Christine Sarai Urbina[1]; Jocelyn Vincent[1]; Saiful Chowdhury[1]; [1]*University 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 Tajdin[1]; Amanda Helms[1]; Jennifer S. Brodbelt[1]; [1]*University 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. Zimmerman[1]; Yunfan Gao[1]; Anne-Lise Marie[1]; Jacqueline Wood[1]; Alexander R. Ivanov[1]; [1]*Barnett 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 Clement[1]; Rajesh K Soni[2]; [1]*Weill Cornell Medicine, New York, NY; [2]Proteomics and Macromolecular Crystallography Shared Resource, Herbert Irving Comprehensive Cancer Center, Columbia University Irving Medical Center, New York, NY, United States, New York, NY*

TP 614 **Phosphoproteomics of MNT-1 Melanoma Cells Reveals Novel Signaling Pathways for Polymyxin B-induced Skin Hyperpigmentation**; Chuhan Zhang[1]; Xiaofen Liu[1]; Jing Zhang[1]; Hailan Wu[1]; Yu Wang[1]; Yaxin Fan[1]; Beining Guo[1]; Xingchen Bian[1]; Xin Li[1]; [1]*Institute 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 Demmers[1]; Karel Bezstarosti[1]; Wouter AS Doff[1]; Lennart Van Der Wal[1]; Karen A Sap[1]; [1]*Erasmus Medical Center Rotterdam, Rotterdam, Netherlands*

TP 616 **Effects of Cold Ischemia on Post-translational Modifications in Patient-Derived Xenograft Models of Cancer**; Keith D. Rivera[1]; Rajan A. Burt[1]; Valentina Cesarani[2]; Natalie M. Clark[1]; D. R. Mani[1]; Jean-Philippe Theurillat[2]; Namrata D. Udeshi[1]; Steven A. Carr[1]; [1]*Broad Institute, Cambridge, MA; [2]Institute of Oncology Research, Bellinzona, Switzerland*

TP 617 **Precision characterization of Phosphorylations Enabled by Individual Ion Mass Spectrometry in MEK1 protein**; Raveena Gupta[1]; Bryon Drown[1]; Jared O. Kafader[1]; John P. McGee[1]; Neil L. Kelleher[1]; [1]*Northwestern University, Evanston, IL*

TP 618 **Tackling citrullination and deamidation challenges in proteomics using high-resolution ion mobility-mass spectrometry (HRIM-MS)**; Heidi Vitrac[1]; Jordan Stewart[1]; Lauren Royer[1]; Ashli Simone[1]; Jesse Meyer[2]; Justyna Fert-Bober[2]; Jennifer Van Eyk[2]; [1]*MOBILion Systems, Chadds Ford, PA; [2]Cedars-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 Zhai[1]; Yepei Huang[1]; Kai Zhang[1]; [1]*Tianjin 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 Prefontaine[1]; Ying Lao[1]; Victor Spicer[1]; Darien Yeung[1]; Nediljko Budisa[1]; Oleg V. Krokhin[1]; [1]*University 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 tumours**; Constance Sobsey[1, 2]; Bjoern C Froehlich[3]; Georgia Mitsa[1, 2]; Arif Awan[4]; Adriana Aguilar-Mahecha[5]; Mark Basik[5]; Christoph H Borchers[1, 4, 6]; Gerald Batist[4, 7]; [1]*Segal Cancer Proteomics Centre, Lady Davis Institute, Jewish General Hospital, Montreal, QC; [2]Division of Experimental Medicine, McGill University, Montreal, QC; [3]CeMOS - Center for Mass Spectrometry and Optical Spectroscopy, Mannheim, Germany; [4]Gerald Bronfman Department of Oncology, McGill University, Montreal, QC; [5]Segal Cancer Centre, Lady Davis Institute, Jewish General Hospital, Montréal, QC; [6]MRM Proteomics Inc., Montréal, QC; [7]Exactis 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 Majedi[2]; Josiane Lafleur[2]; Adriana Aguilar-Mahecha[2]; Rodney Ouellette[4]; Jeremy Roy[4]; Mark Basik[2, 5, 6]; Christoph H. Borchers[1, 3, 7, 8]; [1]*Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [2]Lady Davis*

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TP 624 **Determination of a biomarkers panel to predict the response to treatment with dexamethasone for Sars-Cov2 / COVID-19 pneumonia**; Jerome Vialaret[1]; Christophe Hirtz[1]; Jana Kindermans[1]; Margaux Vignon[1]; Erika Nogue[2]; Nicolas Molinari[2]; Clement Boissin[2]; Jeremy Charriot[2]; *[1]Montpellier Hospital, Proteomics platform (PPC), Montpellier, France; [2]Montpellier 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 Shen[1]; Ming Zhang[1]; Shuo Qian[2]; Sandra R. Montezuma[3]; Deborah A. Ferrington[4]; Jun Qu[1, 5]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell Park Comprehensive Cancer Center, Buffalo, NY; [3]University of Minnesota, Minneapolis, MN; [4]Doheny Eye Institute, Pasadena, CA; [5]New 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 Naicker[2]; Andrea Ellero[3]; Rethabile Mokoena[2, 4]; Justin Jordaan[1]; Stoyan Stoychev[1]; *[1]ReSyn Biosciences, Pretoria, South Africa; [2]Council for scientific and industrial research, Pretoria, South Africa; [3]University of Pretoria, Pretoria, South Africa; [4]University 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 Li[3]; Junghun Lee[1]; Yujung Hwang[3]; Kisoon Dan[1]; Myungwhan Suh[3]; Mookyun Park[3]; Dohyun Han[1, 2]; *[1]Proteomics Core Facility, Transdisciplinary Research and Collaboration, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; [2]Transdisciplinary Department of Medicine and Advanced Technology, Seoul National University Hospital, Seoul, South Korea; [3]Department 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 Park[1]; Kyung-Joo Seong[2]; Se Hwan Jang[1]; Daseul Kim[1]; Ji-Yeon Jung[2]; Won-Jae Kim[2]; Zee-Yong Park[1]; *[1]School of Life Science, Gwangju Institute of Science and Technology, Cheomdangwagiro123, Buk-gu, Gwangju, South Korea; [2]Dental 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 Vajrychova[1]; Jaroslav Stráník[2]; Rudolf Kupčík[1]; Rudolf Kukla[3]; Radka Bolehovská[3]; Marian Kacerovský[2]; *[1]Biomedical Research Center, University Hospital Hradec Kralove, Hradec Kralove, Czech Republic; [2]Department of Obstetrics and Gynecology, University Hospital Hradec Kralove and Faculty of Medicine in Hradec Kralove, Charles University, Hradec Kralove, Czech Republic; [3]Institute 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, Richard[1]; Hangjun Wang[2]; Georgia Mitsa[1]; Olivier Poetz[6]; Margaret Redpath[2]; Andreas Papadakis[2]; Mounib Elchebly[2]; Victor Cohen[7]; Jason Scott Agulnik[7]; Gerald Batist[7]; Alan Spatz[2, 7]; Christoph H. Borchers[1, 2, 7, 8]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [2]Department of Pathology, McGill University, Montreal, QC; [3]Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB; [4]Department of Internal Medicine, University of Manitoba, Winnipeg, MB; [5]Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB; [6]Signatope GmbH, Reutlingen, Germany; [7]Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [8]Division of Experimental Medicine, McGill University, Montreal, QC*

TP 631 **Proteomic predictors of colon tumor distant metastasis**; Anna Wojakowska[1]; Lukasz Marczak[2]; Marcin Zeman[3]; Marta Gawin[3]; Lukasz Skoczylas[3]; Katarzyna Dubkiewicz[2]; Mykola Chekan[4]; Ewa Zembala-Nozynska[3]; Monika Anna Pietrowska[3]; *[1]Institute of Bioorganic Chemistry Polish Academy of Sciences, Poznan, Poland; [2]Institute of Bioorganic Chemistry Polish Academy of Sciences, Poznan, Poland; [3]Maria Sklodowska-Curie National Research Institute of Oncology, Gliwice Branch, Gliwice, Poland; [4]Academy 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 Chen[1]; Lucy Williamson[1]; Margaret Donovan[1]; Purvi Tandel[1]; Gabriel Castro[1]; Taher Elgierari[1]; Aaron S Gajadhar[1]; *[1]Seer, 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 Casavant[1]; Brandon Harder[1]; Manuel Magana[1]; Magdalena Bober[2]; Jakob Vowinckel[2]; W. Rodney Mathews[1]; Veronica Anania[1]; *[1]Genentech, South San Francisco, CA; [2]Biognosys AG, Schlieren, Switzerland*

TP 634 **Automating dwell time determination to increase the efficiency of highly multiplexed SRM method refinement**; Scott Peterman[1]; Alan Atkins[2]; Martin Jech[3]; Abigail Burrows Franco[4]; Scott D Stanley[4]; Neloni Wijeratne[5]; *[1]Thermo Fisher Scientific, Fort Walton Beach, FL; [2]ThermoFisher Scientific, Hemel Hempstead, United Kingdom; [3]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [4]University of Kentucky, Lexington, KY; [5]Thermo 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 Kadayil Prabhakaran[1, 2]; Dijana Vitko[3]; 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]; *[1]Boston Childrens Hospital, Boston, MA; [2]Harvard Medical School, Boston, MA; [3]PrognomiQ Inc, San Mateo, CA*

TP 636 **Integrative proteome analysis for discovery of potential CAR-NK target in TNBC**; Sunghyun Huh[1]; Yourae Shin[1]; Ji Eun Park[1]; Gangsoo Jung[1]; Unbeom Kang[1]; *[1]Bertis 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 Schallenberg[2]; Gabriel Dernbach[2]; Philipp Keyl[2, 3]; Mohamed Haji[1]; Matthias Ziehm[1, 2]; Sylvia Niquet[1, 2]; Christin Beier[1]; Frederick Klauschen[2, 3]; Philipp Mertins[1]; *[1]MDC Berlin, Berlin, Germany; [2]Charité – Universitätsmedizin Berlin, Berlin, Germany; [3]Ludwig-Maximilians-Universität München, Munich, Germany*

TP 638 **Deeper plasma proteome coverage enables identification of novel biomarkers and classification of diseases**; Andreas Schmidt[1]; Katrin Hartinger[2]; Zehan Hu[2]; Claudia Martelli[3]; Katharina Limm[2]; Xaver Wurzenberger[2]; Sebastian Mueller[4]; Nils A. Kulak[2]; [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 Barpanda[1]; Sanjeeva Srivastava[1]; [1]*IIT Bombay, Mumbai, India*

TP 640 **diaPASEF proteomic analysis of human sputum samples for the early diagnosis of lung cancer**; Alejandro Fernández-Vega[1]; María Del Sol Arenas-De Larriva[2]; Bernabé Jurado-Gámez[2]; Ignacio Ortea[3]; [1]*Institute for Biomedical Research and Innovation of Cadiz, Cadiz, Spain;* [2]*Pneumology Unit, Hospital Universitario Reina Sofía, 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 Wai[1]; Ningjian Liang[1]; Bum Jin Kim[1]; Brian Scottoline[2]; David Dallas[1]; [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 Stensballe[1]; Nicolai Bache[2]; Dorte Bekker-Jensen[2]; Mads Lause Mogensen[3]; [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 Casavant[1]; Sumedh Sankhe[2]; Jakob Vowinckel[3]; Nikhil Pandya[2]; Meena Choi[2]; Cecilia Monteiro[2]; W. Rodney Mathews[2]; Veronica Anania[2]; [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 Chang[1]; Yi-Ju Chen[2]; Zhi-Jie Hong[3]; Yi-Jing Hsiao[4]; Guo-Shiou Liao[3]; Sheng-Fang Su[5]; Kuen-Tyng Lin[2]; Huei-Wen Chen[6]; Yen-Shen Lu[7, 8]; Hsuan-Yu Chen[1]; Sung-Liang Yu[4]; Jyh-Cherng Yu[3]; Yu-Ju Chen[2]; [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 Beimers[1]; Noah M Lancaster[2]; Evgenia Shishkova[1]; 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 Su[1]; Alexander R. Ivanov[1]; [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-Teshima[1]; Maiko Okamura[2]; Takashi Nirasawa[3]; Keisuke Hakamada[1]; Tadashi Ikeda[1]; Kozue Murata[1, 4]; Kenji Minatoya[1]; Hidetoshi Masumoto[1, 4]; Masaya Ikegawa[2]; [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 Pulpal Fibroblasts Resulting from Contact with Root Restorative and Pulp-capping Materials**; Mona Goli[1]; Mahmoud Mona[2]; Firas Kobeissy[3]; Roberta Pileggi[2]; Yehia Mechref[1]; [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 Purba[1]; Mona Goli[1]; Chirine El-Baba[2]; Zeinab Ayache[2]; Zeinab Kawtharani[2]; Berthe Hayar[2]; Claudio Pisano[3]; Firas Kobeissy[2, 4]; Nadine Darwiche[2]; Yehia Mechref[1]; [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 Muraoka[1]; Masayo Hirano[1]; Satoshi Nagayama[2]; Junko Isoyama[1]; Mimiko Ishida[1]; Takeshi Tomonaga[1]; 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 Hepburn[1]; Mario E Valdes-Tresanco[1]; Rory Gilliland[1]; Anika Westlund[1]; Annegret Ulke-Lemee[1]; Soren Wacker[1]; Alikhan Mansuri[1]; Gopal Ramamourthy[1]; Thomas Rydzak[1]; Joshua T Smith[2]; Andriy Plakhotnyk[1]; Colin MacKenzie[1]; Maryam Mapar[1]; Bruce J Walker[2]; Ashlee M Earl[2]; Hallgrimur Benediktsson[1]; Daniel B Gregson[1]; M. Ethan McDonald[1]; Ian A Lewis[1]; [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 Weaver[1]; Tristan Finch[1]; Alicia Patrick[1]; Laura Peek[1]; Gary Pestano[1]; [1]*Biodesix, Boulder, CO*

TP 653 **The Role of Native MS in Antibody Research Against Snake Envenoming**; Irina Oganesyan[1]; Julian A. Harrison[2]; Ledsgaard Jensen Line[3]; Cecilie Knudsen[3, 4]; Timothy Patrick Jenkins[3]; Andreas H. Laustsen-Kiel[3, 4]; Renato Zenobi[2]; [1]*ETHZ, Zürich, Switzerland;* [2]*ETH Zurich, Zurich, Switzerland;* [3]*Technical University of Denmark, Kongens*

Lyngby, Denmark; [4]VenomAid 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 Chevreux[1]; Laurent Lignieres[1]; Véronique Legros[1]; Manel Khelil[1]; Nicolas Senecaut[1]; Matthew A Lauber[2]; Jean-Michel Camadro[1]; *[1]Institut Jacques Monod, PARIS, France; [2]Waters 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 Adair[1]; Ian Jones[2]; Rainer Cramer[1]; *[1]Department of Chemistry, University of Reading, Reading, United Kingdom; [2]School 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 Kamal[1]; Jake T Kline[1]; Kenneth R Durbin[2]; Konstantin O Nagornov[3]; Yury O Tsybin[3]; Luca Fornelli[1]; *[1]University of Oklahoma, Norman, OK; [2]Proteinaceous, Evanston, Illinois; [3]Spectroswiss, Lausanne, Switzerland*

TP 657 **FLASHDeconvQ: a software tool for proteome-wide label-free quantification of proteoforms in top-down proteomics**; Jihyung Kim[1]; Kyowon Jeong[1]; Konrad Winkels[2]; Philipp T. Kaulich[2]; Andreas Tholey[2]; Oliver Kohlbacher[1]; *[1]University of Tübingen, Tübingen, Germany; [2]Christian-Albrechts-Universität zu Kiel, Kiel, Germany*

TP 658 **FLASHIda:deep - Historically informed data acquisition in top-down LC-MS/MS batch runs**; Kyowon Jeong[1]; Philipp T. Kaulich[2]; Konrad Winkels[2]; Jihyung Kim[1]; Andreas Tholey[2]; Oliver Kohlbacher[1]; *[1]University of Tübingen, Tuebingen, Germany; [2]Christian-Albrechts-Universität zu Kiel, Kiel, Germany*

TP 659 **A new proteomics data analysis software for top-down mass spectrometry**; George Alevizos[1]; Mariangela Kosmopoulou[1]; Athanasios Smyrnakis[1]; Dimitris Papanastasiou[1]; *[1]Fasmatech, NCSR Demokritos, Athens, Greece*

TP 660 **VUV photodissociation using a diffuse light source integrated in the Omnitrap platform**; Athanasios Smyrnakis[1]; Mariangela Kosmopoulou[1]; Dimitris Papanastasiou[1]; *[1]Fasmatech, NCSR Demokritos, Athens, Greece*

TP 661 **False discovery rate estimation in spectral deconvolution in top-down proteomics**; Ayesha Feroz[1]; Kyowon Jeong[1, 2]; Konstantin Nagornov[3]; Jihyung Kim[1, 2]; Timo Sachsenberg[1, 2]; Yury O. Tsybin[3]; Oliver Kohlbacher[1, 2, 4]; *[1]Applied Bioinformatics, Department for Computer Science, University of Tübingen, Sand 14, 72076, Tübingen, Germany; [2]Institute for Bioinformatics and Medical Informatics, University of Tübingen, Sand 14, 72076, Tübingen, Germany; [3]Spectroswiss, 1015, Lausanne, Switzerland; [4]Translational 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 Le[1]; Patrick Pribil[1]; Yves Le Blanc[2]; *[1]SCIEX, Concord, ON; [2]SCIEX, 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 Wang[1]; Fei Fang[1]; Liangliang Sun[1]; *[1]Michigan 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. Early[1]; Taojunfeng Su[1]; Ryan T. Fellers[1, 2]; Neil L. Kelleher[1]; Kenneth R. Durbin[1, 2]; *[1]Northwestern University, Evanston, IL; [2]Proteinacous, 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 Beloborodov[1]; Pavel Ryumin[1]; Wen Jin[1]; Bradley Schneider[1]; Bill Lloyd[2]; *[1]SCIEX, concord; [2]SCIEX, Concord, ON*

TP 666 **Leveraging intrachain disulfide bonds in proteins for improved sequence coveragein EAD top-down analysis**; Wen Jin[1]; Pavel Ryumin[1]; Lyle L. Burton[1]; *[1]SCIEX, Concord, ON*

TP 667 **Real-Time Spectrum Generation and Online Parameter Optimization During Individual Ion Mass Spectrometry Acquisition**; Ryan T. Fellers[1]; Michael A. R. Hollas[1]; Bryan P. Early[1]; Joseph B. Greer[1]; John P. McGee[1]; Kenneth R. Durbin[2]; Jared O. Kafader[1]; Neil L. Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Proteinaceous, 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 Choi[1]; Geul Bang[1]; Kun Cho[1]; Hyun Joo An[2]; Heeyoun Hwang[1]; *[1]Korea Basic Science Institute, Cheongjusi, South Korea; [2]Graduate 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 Zenaidee[1]; Tyren M Dodgen[2]; Gene Hart-Smith[1]; Luke Carroll[3]; *[1]Australian Proteome Analysis Facility, Macquarie University, Sydney, Australia; [2]Waters Corporation, Sydney, Australia; [3]Australian Proteome Analysis Facility, Macquarie University, Macquarie Park, Australia*

TP 670 **Internal fragmentation generates progressively smaller terminal fragments in top-down mass spectrometry**; Novera Alam[1]; Somak Ray[1]; Jeffrey N Agar[1]; *[1]Northeastern 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 Xu[1]; Liangliang Sun[1]; *[1]Michigan 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 Searfoss[1]; Emily Zahn[1]; Zongtao Lin[1]; Francisca N. de Luna Vitorino[1]; Benjamin A Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

TP 673 **Heavy peaks -examples of qualitative and quantitative potential of intact protein LC-MS**; Waltteri Hosia; *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 Zhao[1]; Yanting Guo[1]; Kellye A Cupp-Sutton[1]; Lushuang Huang[1]; Si Wu[1]; *[1]Oklahoma University, Norman, OK*

TP 675 **Assessing alternative proteases for quantitative proteomics**; Meital Kupervaser[1]; David Morgenstern[1]; Corine Katina[1]; Yishai Levin[1]; *[1]The 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 McGann[1]; William Barshop[2]; Jesse Canterbury[2]; Chuwei Lin[3]; Thomas Perkins[3]; David Bergen[2]; Jingjing Huang[2]; Graeme McAlister[2]; Devin Schweppe[3]; *[1]University of Washington, Seattle, WA; [2]Thermo Fisher Scientific, San Jose, CA; [3]University of Washington, Seattle, WA*

TP 677 **directLFQ, an algorithm for ultra-fast, accurate and open proteomics quantification**; Constantin Ammar[1]; Julia Schessner[1]; Sander Willems[1]; André Michaelis[1];

Matthias Mann[1]; *[1]Max 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 Boujenoui[1]; Mathilde Lahaise[1]; Francis Beaudry[1]; *[1]Universite de Montreal, St-Hyacinthe, QC*

TP 679 **ESI Source Comparison and Optimization on a Capillary-flow SureQuant Assay**; Yi (jimmy) Zeng[1]; Ruby Karimjee[1]; Sara Nouri Gomaei[1]; Hao Qian[1]; Esthelle Hoedt[1]; Joon-Yong Lee[1]; Philip Ma[1]; Bruce Wilcox[1]; *[1]PrognomiQ 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 Xavier[1]; Keith Ashman[2]; Peter G Hains[1]; Phillip J Robinson[1]; *[1]ProCan®, Children's Medical Research Institute, Faculty of Medicine and Health, The University of Sydney, Westmead, Australia; [2]SCIEX, Sydney, Australia*

TP 681 **High-throughput sample preparation workflow for absolute quantitative proteomics combining cell-free QconCAT synthesis and in-StageTip digestion**; Ayako Takemori[1]; Ryo Konno[2]; Yusuke Kawashima[2]; Yuto Hamazaki[3]; Ayuko Hoshino[3]; Nobuaki Takemori[1]; *[1]Ehime University, Toon, Japan; [2]Kazusa DNA Research Institute, Kisarazu, Japan; [3]Tokyo 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, Richard[1]; Georgia Mitsa[1, 2]; Daria Chaplygina[1]; Mario Thevis[3, 4]; Christoph H. Borchers[1, 2, 5, 6]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [2]Division of Experimental Medicine, McGill University, Montreal, QC; [3]Institute of Biochemistry, Center for Preventive Doping Research, German Sport University, Cologne, Germany; [4]European Monitoring Center for Emerging Doping Agents (EuMoCEDA), Cologne/Bonn, Germany; [5]Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [6]Department of Pathology, McGill University, Montreal, QC*

TP 684 **Enhanced TMT data analysis with AI-driven workflows utilizing CHIMERYS and INFERYS algorithms**; Mick Greer[1]; Mark Sanders[2]; David M Horn[3]; Kai Fritzemeier[4]; *[1]Thermo Fisher Scientific, Austin, TX; [2]ThermoFisher Scientific, Somerset, NJ; [3]ThermoFisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

TP 685 **Discovery and validation of "missing human proteins" based on analysis of gastric cancer tumor cells**; Yining Cai[1]; Chunhui Gu[1]; Fuchung Hsiao[1]; Jennifer B Dennison[1]; Jody Vykoukal[1]; Johannes Fahrmann[1]; Kim-Anh Do[1]; Shumei Song[1]; Jaffer Ajani[1]; Ehsan Irajizad[1]; Hiroyuki Katayama[1]; Samir Hanash[1]; *[1]University of Texas MD Anderson Cancer Center, Houston, TX*

TP 686 **Developing differential absolute quantification assays for targeted cancer proteogenomics**; Yassene Mohammed[1]; Constantinos Blidjios[2]; Karl Makepeace[3]; Pallab Bhowmick[3]; Vincent R, Richard[4]; Christoph H. Borchers[5, 6, 7, 8]; *[1]Center for Proteomics and Metabolomics, Leiden University, Leiden, Netherlands; [2]Department of Oncology, McGill University, Montreal, QC; [3]University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; [4]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [5]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [6]Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [7]Division of Experimental Medicine, McGill University, Montreal, QC; [8]Department of Pathology, McGill University, Montreal, QC*

TP 687 **Quantitative Proteomic Analysis of Sputum Reveals Proteins Associated with Inflammatory Response to Woodsmoke Exposure**; Angie L Mordant[1]; Christine A Mills[1]; Alexis Payton[2, 3]; Laura E Herring[1]; Neil E Alexis[4]; Heather Wells[4]; David B Peden[4, 5]; Julia Rager[2, 3, 6]; Ilona Jaspers[2, 4, 7]; *[1]UNC Proteomics Core Facility, Department of Pharmacology, University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Department of Environmental Sciences and Engineering, Gillings School of Global Public Health, UNC Chapel Hill, Chapel Hill, NC; [3]Center for Environmental Medicine and Lung Biology, School of Medicine, UNC Chapel Hill, Chapel Hill, NC; [4]Center for Environmental Medicine Asthma and Lung Biology, Department of Pediatrics, UNC Chapel Hill, Chapel Hill, NC; [5]Department of Pediatrics, Division of Allergy & Immunology, UNC Chapel Hill, Chapel Hill, NC; [6]Institute for Environmental Health Solutions, Gillings School of Global Public Health, UNC Chapel Hill, Chapel Hill, NC; [7]Department 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 Deng[1]; Aman Makaju[1]; Daryl Bulloch[2]; Bo Zhou[1]; *[1]Amgen, Thousand Oaks, CA; [2]Amgen, Inc., South San Francisco, CA*

TP 689 **Proteomic Analysis of Six Mammalian Cell Lines Reveals Individual Lysosomal Composition and Novel Lysosomal Proteins**; Sara Bonini[1]; Fatema Akter[1]; Srigayatri Ponnaiyan[1]; Bianca Kögler-Mohrbacher[2]; Florian Bleibaum[3]; Markus Damme[3]; Bernhard Y Renard[2]; Dominic Winter[1]; *[1]Institute for Biochemistry and Molecular Biology, Medical Faculty, Rheinische Friedrich-Wilhelms-University of Bonn, Bonn, Germany; [2]Bioinformatics Unit (MF1), Robert Koch Institute, Berlin, Germany; [3]Institute for Biochemistry, Kiel, Germany*

TP 690 **TMT quantitative proteomics of bortezomib treated cell line models of AL amyloidosis and multiple myeloma**; Gary Bradshaw[1]; Cameron S Fraser[1, 2, 3]; Marian Kalocsay[4]; Kristopher Sarosiek[1, 2, 3]; *[1]Laboratory of Systems Pharmacology, Boston, MA; [2]John B. Little Center for Radiation Sciences, Harvard TH Chan School of Public Health, Boston, MA; [3]Program in Molecular and Integrative Physiological Sciences, Harvard TH Chan School of Public Health, Boston, MA; [4]Department 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 subtropicaATCC 51142 proteome**; Punyatoya Panda[1]; Uma K Aryal[1]; *[1]Purdue University, West lafayette, Indiana*

TP 692 **Systemized proteomics by automating the TMT global protein profiling workflow**; Taylur P Ma[1]; Hanna G Budayeva[2]; Kristan Bahten[3]; Beibei Huang[4]; Maowei Dou[3]; *[1]Genentech, Inc., South San Francisco, CA; [2]Genentech Inc, South San Francisco, CA; [3]ThermoFisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, San Jose, CA*

TP 693 **Enabling high depth proteomic analysis of rat plasma through comparison of depletion strategies**; Jan Muntel[1]; Theresa Keil[1]; Christin Zasada[1]; Janine Sequeira[1]; Marsilio Adriani[2]; Krzysztof Okrasa[2]; Hannes Hahne[1]; *[1]OmicScouts, Freising, Germany; [2]Sosei Heptares, Cambridge, United Kingdom*

TP 694 **Proteomic characterization of Oreochromis niloticus skin used as a biological dressing**; Iasmim Lopes De Lima[1]; Cláudia B. A. Medeiros[2]; Isabella Cavalcanti[2]; Fabricio Oliveira Souto[2]; Marcos Nogueira Eberlin[1]; Roberto Afonso Da Silva[2]; Marcelo Borges Miranda[3]; José Luiz Lima Filho[2]; *[1]MackMass Laboratory, Mackenzie Presbyterian University, São Paulo, Brazil; [2]Keizo Asami Institute,* *Federal University of Pernambuco, Recife, Brazil; [3]São Marcos Hospital/Rede D'Or, Recife, Brazil*

TP 695 **Deep proteome profiling of breast implant capsules with contracture shows high burden of inflammatory processes**; Ole Østergaard[1]; Andreas Larsen[2]; Tim Kongsmark Weltz[2]; Mikkel Herly[3]; Jesper Velgaard Olsen[1]; *[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 Tran[1]; Gaoyuan Lu[1]; Wenxin Wu[2]; Thao Duong[2]; 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 Yu[1]; Liping Yao[1]; Yang Li[1]; Hong Chen[1]; Chenghao Situ[1]; Zhibin Hu[1]; Xuejiang Guo[1]; *[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 Situ[1]; Weiling Yu[1]; Hong Chen[1]; Liping Yao[1]; Xiangzheng Zhang[1]; Xuejiang Guo[1]; *[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 Neuenroth[1]; Jumana Jaber[1]; Verena Ebner[1]; 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 Centre 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 Zaman[1]; Autumn B Morgan[2]; Vien Nguyen[1]; Katalin Prokai-Tatrai[1]; Denise M Inman[2]; Laszlo Prokai[1]; *[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. Najjar[1]; Yulanda M. Williamson[2]; Paul J. Branham[1]; Hans C. Cooper[2]; John R. Barr[2]; Tracie L. Williams[2]; *[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 Zhang[1]; William E. Wallace[1]; Guanghui Wang[1]; Meghan C. Burke Harris[1]; Yi Liu[1]; Sergey L. Sheetlin[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

TP 703 **Spatially-resolved proteomics of drug-dosed tissue by use of liquid extraction surface analysis**; Peter Macey[1]; Iain B. Styles[1]; Helen J. Cooper[1]; *[1]University of Birmingham, Birmingham, United Kingdom*

TP 704 **Differential proteomics to probe molecular basis for a renal phenotype associated with GPR110 deletion**; Bill Huang[1]; Karl Kevala[1]; Hee-Yong Kim[1]; *[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 Khan[1]; Valentina Marassi[2]; Barbara Roda[2]; Cristina C. Clement[1]; *[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 Camporesi[1]; Amal Kasri[2]; Gunnar Brinkmalm[3]; Marie-Claude Potier[2]; Henrik Zetterberg[3]; Eleni Gkanatsiou[1]; Lev Stimmer[4]; Andre Strydom[5]; Yannick Vermeiren[6]; *[1]Gothenburg University, Gothenburg, Sweden; [2]Institute du Cerveau-CNRS UMR7225-Inserm U1127-UPMC, Hopital de la Pitié-Salpetriére 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 Inns[1]; José Luis Marín-Rubio[1]; Matthias Trost[1]; Neil Rajan[1]; *[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 Collins[1]; Taufika Islam Williams[1]; Andreea Biehl[1, 2]; Ana Gracioso Martins[1, 2]; Zachary Davis[1, 2]; Daphne Sze[1, 2]; Camilo Mora-Navarro[3]; 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. Prokai[1]; Khadiza Zaman[2]; Vladimir Shulaev[1]; *[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 Jani[1]; Olivier Duverger[1]; Marian Young[1]; Lee Jannice[1]; Yan Wang[1]; *[1]NIH/NIDCR, BETHESDA, MD*

TP 711 **SYSTEMS BIOLOGY OF ATHEROSCLEROTIC HUMAN CAROTID ARTERIES THROUGH MASS SPECTROMETRY-BASED PROTEOMICS**; Laszlo Prokai[1, 2]; Éva Csősz[2]; Gergő Kalló[2]; Ajnees Kumar[2]; Khadiza Zaman[1]; Uladzislau Vadadokhau[2]; László Potor[2, 3]; Zoltán Hendrik[2]; Gábor Méhes[2]; Csaba Tóth[2]; Péter Gergely[2]; József Tőzsér[2]; György Balla[3]; 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 FFPE Tumor Tissue**; Andrew Chambers[1]; Steve Sweet[1]; Zifeng Song[1]; David Chain[1]; Claire Rooney[2]; Yeoun Jin Kim[1]; *[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 Greenwald[1]; Paola Loreto Palacio[2]; Yongseok Kim[1]; Setty M Magaña[2]; Vicki H Wysocki[1]; *[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*

TP 714 **Poly[n]rotaxanes: From Synthesis To Mass Spectrometric Characterizations**; Bo Song[1]; James Seale[1]; Yunyan Qiu[2]; Fraser Stoddart[1]; [1]*Northwestern University, Evanston, IL;* [2]*National University of Singapore, Singapore, Singapore*

TP 715 **Detecting Oxygen Inhibition in Adhesive Systems Using ASAP-MS**; Christopher Joseph Shaffer[1]; Spencer Johnson[2]; Dana Reed[1]; Amanda Leone[1]; Wayne Mahoney[1]; Eric Nelson[1]; [1]*3M, Saint Paul, MN;* [2]*Brigham Young University, Provo,, UT*

TP 716 **Dissecting Complex Polymer Mass Spectra by Fourier Transform-based Deconvolution and Macromolecular Mass Defect Analysis**; Andrew K Swansiger[1]; Christopher M. Crittenden[2]; Rekha Thomas[2]; James S Prell[1, 3]; Bifan Chen[2]; [1]*University of Oregon, Eugene, OR;* [2]*Genentech Inc, South San Francisco, CA;* [3]*Materials Science Institute, University of Oregon, Eugene, OR*

TP 717 **Investigation of fluoropolymersby Thermodesorption/Pyrolysis-DART coupled to very high-resolution mass spectrometry**; Pierre Pacholski[1, 2]; Frédéric Progent[1]; Sébastien Schramm[2]; Frédéric Aubriet[2]; [1]*CEA, DAM, DIF, F-91297 Arpajon, France;* [2]*Laboratoire 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 Nissinen[1]; Krista Gronlund[1]; Janne Janis[1]; Jarkko J. Saarinen[1]; Mika Suvanto[1]; Ilkka Rytoluoto[2]; Jani Pelto[2]; [1]*University of Eastern Finland, Department of Chemistry, Joensuu, Finland;* [2]*VTT Technical Research Centre of Finland Ltd., Tampere, Finland*

TP 719 **Combining IMS with MS/MS for Accelerated Readout of Digital Polymers**; Isaure Sergent[1]; Thibault Schutz[2]; Laurence Oswald[3]; Jean-François Lutz[2]; Laurence Charles[1]; [1]*Aix Marseille Université, CNRS, Institut de Chimie Radicalaire, MARSEILLE, France;* [2]*Université de Strasbourg, CNRS, UMR 7006, Institut de Science et d'Ingénierie Supramoléculaires, Strasbourg, France;* [3]*Université 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 Patil[1]; Thị Khánh Ly Lại[1]; Wen-Ping Peng[1]; [1]*National Dong Hwa University, Shoufeng, Taiwan*

TP 721 **>10,000 Da polymer detection using Q ExactiveTM UHMR: In-Source Trapping and Charge Reduction**; Junho Jeon[1]; Anthony Gies[1]; Zoltan Szabo[2]; Katie Peterson[2]; [1]*The Dow Chemical Company, Lake Jackson, TX;* [2]*Thermo 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 Ackerman[1]; Kristen L Reese[1]; Jānis Ruško[2]; Ingus Pērkons[2]; [1]*FDA Center for Food Safety, College Park, MD;* [2]*Institute 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 Liu[1]; Feixue Wang[1]; Li Fang[1]; Peiyun An[1]; Jinlian Lu[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; [1]*WuXi AppTec, Shanghai, China*

TP 724 **Waters RADIANTM ASAP Probe: Industrial Application of a ASAP Direct Mass Detector and a UHR-MS ASAP**; Janece Potter[1]; Junho Jeon[1]; Anthony Gies[1]; Bryan Katzenmeyer[2]; [1]*Dow, Inc., Lake Jackson, TX;* [2]*Waters Corporation, Milford, MA*

TP 725 **NP-SIMS as a tool for evaluating the homogeneity of extreme-ultraviolet resists**; Jander Cruz[1]; Stanislav Verkhoturov[2]; Emile A. Schweikert[2]; Michael Eller[1]; [1]*California State University Northridge, Northridge, CA;* [2]*Texas 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]; [1]*State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, Hong Kong SAR, China;* [2]*Department of Chemistry, Hong Kong Baptist University, Hong Kong, China;* [3]*State 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;* [4]*EIT 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 Yeo[1]; Reji N Nair[1]; Ayodele O Ogunkoya[1]; Xiao Cai[1]; Stepan Chuprakov[1]; Robyn M Barfield[1]; Maxine Bauzon[1]; Tiffany Unsulangi[1]; Jesus Aguilar[1]; Thomas Linz[1]; Jia Yang[1]; Fangjiu Zhang[1]; Alyssa G Occiano[1]; Dharmaraj Samuel[1]; Penelope M Drake[1]; [1]*Catalent 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 Griffeuille[1]; Sylvain Dulaurent[1]; Souleiman El Balkhi[1]; Stephane Moreau[2]; Franck Saint-Marcoux[1]; [1]*CHU Limoges, Limoges, France;* [2]*SHIMADZU Europe, Cugnaux, France*

TP 729 **Harmful textile chemicals - Investigation of dermal uptake and peptide modifications in reconstructed human epidermis**; Josefine Carlsson[1]; Pablo Pardo Menacho[1]; Conny Ostman[1]; Ulrika Nilsson[1]; [1]*Stockholm 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 Jenkins[1]; Elizabeth Dhummakupt[2]; Gabrielle Rizzo[2]; Allison Melka[3]; Dylan Fudge[2]; Tyler Goralski[2]; [1]*U.S. Army DEVCOM CBC, APG, MD;* [2]*U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD;* [3]*EXCET Incorporated, Edgewood, MD*

TP 731 **Drugs of abuse in hair: high speed and sensitivity demands for LC-MS/MS**; Ichiro Hirano[1]; Marcos Pudenzi[2]; Luis Otavio Junqueira[2]; [1]*Shimadzu do Brasil Comercio Ltda, Barueri, Brazil;* [2]*Shimadzu 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 Feng[1]; Ili Erdemir[1]; Lei Zhu[1]; Matthew Kuhls[1]; Wen Kang[1]; Nianyu Li[1]; Raymond Gonzalez[1]; Kara Pearson[1]; [1]*Merck & 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 Åström[1]; Maria Ximena Ruiz Caldas[2]; Ioannis Sadiktis[2]; Ulrika Nilsson[2]; Aji P Mathew[2]; [1]*Stockholm University, Stockholm, Sweden;* [2]*Stockholm 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

Ambient Ionization: Applications I	001-020
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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. Beach[3]; 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 Pereira[1]; Joseph Monaghan[1, 2]; Lucas R. Abruzzi[1, 2]; Jason L. Robinson[3]; 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 McKeown[1]; Jian Yu[1]; Richard Oleschuk[1]; *[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 Fedick[1]; Ryan M Bain[2]; Tj Pinedo[1]; Christopher C. Mulligan[3]; Douglas J. Klapec[2]; *[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. Emmons[1]; Aghogho A. Olomukoro[1]; William L. Fatigante[2]; Brian Musselman[2]; Emanuela Gionfriddo[1]; *[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 Cody[1]; Krishnaja Tikkisetty[2]; Paige McCallum[2]; Taylor Filewood[2]; Jeffrey Yan[2]; Honoria Kwok[2]; Pamela Brunswick[2]; Dayue Shang[2]; *[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 Kooij[1]; Cees Van Rijn[1]; Neil Ribe[2]; Daniel Bonn[1]; *[1]Van der Waals Zeeman Institute, Amsterdam, Netherlands; [2]1Lab 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 Chen[1]; Evan R. Williams[1]; *[1]University of California Berkeley, Berkeley, CA*

WP 010 **Silica nanoparticles induce oxidative stress as measured by mass spectrometry**; Yangjie Li[1]; Kurt W. Kolasinski[2]; Richard N Zare[1]; *[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-Federle[1]; Nicholas Manicke[1]; *[1]Indiana University Purdue University Indianapolis, Indianapolis, IN*

WP 012 **PGE2 is localized outside the COX2 positive implantation site during pregnancy**; Joanne B Ballantyne[1]; Thanai Paxton[2]; Yuri Sugiura[3]; Rae Maeda[3]; *[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

Bonose[1]; Ayoub Boulghobra[2]; *[1]Université Paris saclay, Gif sur Yvette, France; [2]Université Paris saclay, orsay, France*

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 Gasilova[1]; Daniel Trujillo Ortiz[1]; Laure Menin[1]; *[1]EPFL SB ISIC-GE, Lausanne, Switzerland*

WP 015 **Real time volatile sulfur compounds monitoring using DART ion source**; Motoshi Sakakura[1]; Teruhisa Shiota[1]; Yasuhiko Bando[1]; *[1]AMR Inc., Meguro-Ku, Japan*

WP 016 **Polymeric Surface Modification of Swabs for Enhanced Detection of Lipids Using High Throughput DESI-MS**; Elmeri Latvanen[1]; Maria Sani[1]; Dani Simon[1]; Alva Si[1]; Yuchen Xiang[1]; Vincen Wu[1]; Petra Paizs[1]; James Kinross[1]; Panagiotis Manesiotis[2]; Zoltan Takats[1]; Lauren Ford[1]; *[1]Imperial College London, London, United Kingdom; [2]Queen's University Belfast, Belfast, United Kingdom*

WP 017 **Heterogeneous Catalysis by Fullerene C-60: Photocatalytic Dehydro-Dimerization of Primary Amines and Tetrahydroquinolines**; Savithra Jayaraj[1]; Kavyasree Chintalapudi[1]; Abraham Kwame Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

WP 018 **Temperature Profiling and Quantitative Analysis of Disperse Dyes in Polyester via DART Mass Spectrometry**; Zoe J Millbern; *NC 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 Arao[1]; Yuta Miyazaki[1]; Natsuyo Asano[1]; Hidenori Takahashi[1]; *[1]SHIMADZU 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 Lu[1]; Chao-Xuan Zhang[1]; Patrick Rodrigues[1]; Lei Yang[1]; Aaron Shafer[1]; Frank Fazio[1]; *[1]St. Jude Children's research hospital, Memphis, TN*

WP 021 **Improved Biopharmaceutical Peptide Mapping Workflows Using a Novel Autolysis-Resistant Trypsin Enzyme**; Samantha Ippoliti[1]; Nick Zampa[1]; Ying Qing Yu[1]; Matthew A Lauber[1]; *[1]Waters 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 Röwer[1]; Oladapo Olaleye[2]; Rainer Bischoff[2]; Michael O. Glocker[1]; *[1]Proteome Center Rostock, Rostock, Germany; [2]Department 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 Hwang[1]; Hyejin Kim[2]; Geul Bang[1]; Hyun Joo An[3]; Jong Shin Yoo[1]; Jin Young Kim[1]; Yeseul Park[4]; *[1]Korea Basic Science Institute, cheongju, South Korea; [2]Korea Advanced Institute of Science and Technology, Daejeon, South Korea; [3]Chungnam National University, Daejeon, South Korea; [4]Korea Basic Science Institute, Cheongju, South Korea*

WP 024 **Ex vivo mass spectrometry-based biodistribution of total antibody and released payload of an ADC**; Domenico Ravazza[1]; Lucrezia Principi[1]; Lydia Bisbal Lopez[2]; Andrea Galbiati[1]; Aureliano Zana[1]; Matilde Bocci[1]; Sheila Dakhel[1]; Samuele Cazzamalli[1]; Dario Neri[3, 4]; Alberto Dal Corso[2]; Ettore Gilardoni[1]; *[1]Philochem AG, Otelfingen, Switzerland; [2]Chemistry Department, Università degli studi di Milano, Milan, Italy; [3]ETH Zurich, Zurich, Switzerland; [4]Philogen S.p.A., Sovicelle, Italy*

WP 025 **Comparison of glycopeptide and released N-glycan abundances for IgG-based therapeutic antibodies**; Concepcion Africano Remoroza[1]; Meghan C. Harris-Burke[1]; Tytus D. Mak[1]; Brian T. Cooper[1, 2]; Zachary C. Goecker[1]; Sergey L. Sheetlin[1]; Yuri A. Mirokhin[1]; Guanghui Wang[1]; Xiaoyu Yang[1]; Dmitrii V. Tchekhovskoi[1]; Stephen E. Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]University 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 Zhu[1]; Min Ma[2]; Ming Zhang[1]; Jun Qu[1, 3]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell Park Comprehensive Cancer Center, Buffalo, NY; [3]New 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 Šiborová[1]; Douwe Schulte[1]; Joost Snijder[1]; *[1]Utrecht University, Utrecht, Netherlands*

WP 028 **Comprehensive Biotransformation Analysis of a DAR4 ADC using Intact LC-HRMS from in vivo Cynomolgus Monkey Samples**; Hui Yin Tan[1]; Yue Huang[1]; Jiaqi Yuan[1]; Anton I. Rosenbaum[1]; *[1]AstraZeneca, South San Francisco, CA*

WP 029 **Multi-specific construct separation using native reversed-phase liquid chromatography**; Shuai Wu[1]; Aniruddha Sahasrabuddhe[1]; Wenchao Sun[1]; *[1]Amgen Inc., Thousand Oaks, CA*

WP 030 **Charge heterogeneity characterization and peak identification of complex protein therapeutics using an icIEF-UV/MS system**; Mingjie Cui[1]; Kristin Schultzkuszak[1]; Trust Razunguzwa[1]; Weiguo Zhai[1]; Scott Mack[2]; Jingwen Ding[2]; Zoe Zhang[2]; Maggie Ostrowski[2]; *[1]AstraZeneca, Gaithersburg, MD; [2]SCIEX, Fremont, CA*

WP 031 **Paper-Based Immunoassay for Multiplexed Detection of Colorectal Cancer Biomarkers Through Direct Paper Spray Mass Spectrometry**; Girish Muralikrishnan[1]; Abraham Kwame Badu-Tawiah[1]; *[1]The 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 Kosanam[1]; George Perkins[1]; Jared Kress[1]; Haichuan Liu[2]; Eshani Nandita[2]; Zoe Zhang[2]; *[1]Merck & Co., Inc., West Point, PA; [2]SCIEX, 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 Li[1]; Rosendo Villafuerte-Vega[1]; Thomas R. Slaney[2]; Naresh Chennamsetty[2]; Guodong Chen[2]; Li Tao[2]; Brandon T Ruotolo[1]; *[1]University of Michigan, Ann Arbor, Michigan; [2]Bristol 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. Dykstra[1]; Heidi Vitrac[2]; Thomas Lubinsky[2]; Ashli Simone[2]; Iain D. G. Campuzano[1]; Pavel Bondarenko[1]; *[1]Amgen, Thousand Oaks, CA; [2]MOBILion 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 Liu[1]; Andrew Mahan[2]; Hirsh Nanda[2]; Elliott Jones[1]; Zoe Zhang[1]; *[1]SCIEX, Redwood city, CA; [2]Janssen, Spring House, PA*

WP 036 **Efficient and sensitive peptide mapping approach by μPAC columns with ultralow sample loading**; Yuan Lin[1]; Xuefei Sun[1]; Jeff Op De Beeck[2]; Shanhua Lin[1]; *[1]Thermo Fisher Scientific, Sunnyvale, CA; [2]Thermo Fisher Scientific, Ghent, Belgium*

WP 037 **Utilizing HRAM Orbitrap MS to Quantify Therapeutic Monoclonal Antibodies in Human Serum for Clinical Research**; Yvonne Ehwang Song[1]; Stephanie N. Samra[1]; Kerry Hassell[1]; Julia Poncher[1]; Bradley Hart[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

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) Xue[1]; Emily Williamson[1]; Daniel Skrocki[1]; Min Meng[2]; Aihua Liu[1]; *[1]Alliance Pharma, Malvern, PA; [2]Chongqing Denali Medpharma Co.,Ltd, Chongqing, China*

WP 039 **LC-MS Characterization of Multi-Specific Antibodies**; Jeremy Wolff[1]; Vera B. Ivleva[1]; Yile Li[1]; Melissa Resto[1]; Jason G. Gall[1]; Q. Paula Lei[1]; *[1]NIH, Gaithersburg, MD*

WP 040 **Conformation of Native Antibody-Drug Conjugate Charge Variants Revealed by Microchip Capillary Electrophoresis Coupled with Trapped Ion Mobility**; Eli J Larson[1]; Adi M Kulkarni[2]; Jake A Melby[3]; Matthew Fischer[3]; Zhan Gao[4]; Kevin M. Buck[3]; Melissa R. Pergande[4]; Yanlong Zhu[5]; Guillaume Tremintin[6]; Kate Yu[2]; Ying Ge[3, 4, 5]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]908 Devices, Inc., Boston, MA; [3]Department of Chemistry, University of Wisconsin - Madison, Madison, WI; [4]Department of Cell and Regenerative Biology, University of Wisconsin - Madison, Madison, WI; [5]Human Proteomics Program, University of Wisconsin - Madison, Madison, WI; [6]Bruker Daltonics, San Jose, CA*

WP 041 **Rapid identification of conjugation sites in antibody drug conjugates using Microchip Capillary Electrophoresis Coupled with Mass Spectrometry**; Yue Ju[1]; Adi M Kulkarni[2]; Hampus Engstroem[2]; Erin Redman[2]; Kate Yu[2]; Guillaume Tremintin[1]; *[1]Bruker Daltonics, San Jose, CA; [2]908 Devices, Inc., Boston, MA*

WP 042 **Analyses of chemical modifications in therapeutic antibodies by high resolution multi-turn TOF-MS system**; Yusuke Tateishi[1]; Hiroyuki Miura[1]; Hiroko Morinaga[1]; Koichi Kimura[1]; Tetsuo Iida[1]; Junna Nakazono[1]; Masaru Nishiguchi[1]; Osamu Furuhashi[1]; Daisuke Okumura[1]; Yuki Yamaguchi[2]; Susumu Uchiyama[2]; *[1]SHIMADZU Corporation, Kyoto, Japan; [2]Osaka Univerisity, Suita, Osaka, Japan*

WP 043 **Improved intact antibody characterization with a new ion source design**; Kilian Mayr[1]; Daniel Jajcevic[1]; Lauren Stempfl[1]; Christian Albers[2]; Dodge Baluya[3]; José Bonfiglio[1]; Rebekka Kroiher[1]; Annette Vogt[1]; *[1]Roche Diagnostics GmbH, Penzberg, Germany; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bruker 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. Vieira[1]; Aditya Kulkarni[2]; Kate Yu[2]; Peiyi Shen[1]; Pei-Ni Tsai[1]; Timothy Weeden[1]; *[1]Dyne Therapeutics, Inc., Waltham, MA; [2]908 Devices, Inc., Boston, MA*

WP 046 **Structural Characterization of Biopharmaceutical Proteins using Ion-Mobility and Collision Induced Unfolding**; Kristine F Parson[1]; Margo Wilson[1]; Hunter Walker[1]; Greg Adams[1]; *[1]FUJIFILM Diosynth Biotechnologies USA, Morrisville, NC*

WP 047 **Sensitive bioanalysis of galactosylsphingosine (GalSPH) and glucosylsphingosine (GluSPH) in cerebral spinal fluid**; Kean Woodmansey[1]; Jack Steed[1]; Jessica Smith[1]; Freddy Oostebring[2]; Jianru Stahl-Zeng[3]; *[1]SCIEX, Macclesfield, United Kingdom; [2]Ardena Bioanalysis, Assen, Netherlands; [3]SCIEX, Darmstadt, Germany*

WP 048 **5-Lipoxygenase Clinical Biomarker Method Development – Overcoming Selectivity, Stability, and Reagent Resourcing Challenges**; Liu Yang[1]; John Meissen[1]; Elske Franssen[2]; Anton I. Rosenbaum[1]; *[1]Integrated Bioanalysis, Clinical Pharmacology & Safety Sciences R&D, AstraZeneca, South San Francisco, CA; [2]Translational 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 Popp[1]; Aaron S. Gajadhar[3]; Paul Pease[3]; Lucy Williamson[4]; Asim Siddiqui[4]; Christoph H. Borchers[5, 6, 7, 8]; *[1]MRM Proteomics Inc., Montréal, QC; [2]Département de Biomédecine Vétérinaire, Faculté de Médecine Vétérinaire, Université de Montréal, Saint-Hyacinthe, QC; [3]Seer Inc., Redwood City, CA; [4]Seer, Inc., Redwood City, CA; [5]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [6]Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [7]Division of Experimental Medicine, McGill University, Montreal, QC; [8]Department of Pathology, McGill University, Montreal, QC*

WP 050 **Quantitative Glycoproteomic Analysis of High-Density Lipoproteins in Alzheimer's Disease using LC-MS/MS**; Armin Oloumi[1]; Brian Hong[1]; Yasmine Bouchibti[1]; Michael Russelle S. Alvarez[1]; Angela M. Zivkovic[1]; Carlito B. Lebrilla[1]; *[1]UC 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 Huo[1]; Shichen Shen[1]; Ming Zhang[1]; Jun Qu[1, 2]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell 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 Ubhayasekera[1]; Jonas Bergquist[2]; *[1]Uppsala University, Uppsala, Sweden; [2]Uppsala 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 Lehmann[2]; Christophe Hirtz[2]; Jerome Vialaret[2]; *[1]Shimadzu France, Noisiel, France; [2]IRMB-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 Roger[3]; Andree Schmidt[4, 5]; Cerina Chhuon[6]; Stefan Breimann[4, 5]; Joanna Lipecka[7]; Sophie Dreux[8]; Mueller Stefan[4, 5]; Michel Zerah[9]; Jerome Larghero[9]; Jean-Marie Jouannic[1]; Stefan Lichtenthaler[4, 5]; Chiara Guerrera[7]; *[1]Sorbonne 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; [2]Paris University, Stem Cell Biotechnologies Unit, INSERM 976, CIC-BT CBT501, AP-HP, Saint-Louis Hospital, Paris, France; [3]Proteomics Platform Necker, Paris, France; [4]German Center for Neurodegenerative Diseases (DZNE), Munich, Germany; [5]Neuroproteomics, School of Medicine, Klinikum Rechts der Isar, Technische Universität München, Munich, Germany; [6]Proteomics Platform Necker, Paris, France; [7]Proteomics Platform Necker, Paris, France; [8]Paris University, Biochemistry-Hormonology, AP-HP, Robert Debré Hospital, Paris, France; [9]Paris 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. Cazares[1]; Raghothama Chaerkady[1]; Chiung-Yun Chang[1]; Abby J. Chiang[1]; Helen Killick[2]; Jessica Holmén Larsson[2]; Ian Christopher Scott[2]; Sonja Hess[1];

[1]AstraZeneca R&D, Gaithersburg, Maryland; [2]AstraZeneca, 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 Berthemy[1]; Maud Heuillet[1]; Aude Dupuy-Gayral[1]; Eloi Haudebourg[1]; Catherine Pech[1]; Benoît Souchet[2]; Alkéos Michaïl[2]; Baptiste Billoir[2]; Jérôme Braudeau[2]; François Autelitano[1]; *[1]EVOTEC, Toulouse, France; [2]AgenT, 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 Ji[1]; Yulemni Morel[1]; Anh Tran[1]; Jace W. Jones[1]; *[1]University 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 Pandey[1]; Nageswara Pilli[1]; William Temple Andrews[1]; Ludovic Muller[1]; Maureen Kane[1]; *[1]University of Maryland School of Pharmacy, Baltimore, MD*

WP 059 **Enhanced LC-MS Analysis of Volatile Organic Compound Metabolites in Wastewater**; David Hoetker[1]; Zhengzhi Xie[1]; Pawel Lorkiewicz[1]; Ted Smith[2]; Sanjay Srivastava[3]; *[1]Christina Lee Brown Envirome Institute, University of Louisville, Louisville, KY; [2]Center for Healthy Air Water Soil, University of Louisville, Louisville, KY; [3]Superfund 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 Dee[1]; Christopher M. Shuford[1]; Russell P Grant[1]; *[1]LabCorp, 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 Karnik[1]; Matthew Hartle[1]; Melodie Boute[2]; Richard Ruez[2]; Corinne Ramos[2]; *[1]Pyxant Labs, Inc., Colorado Springs, CO; [2]ImaBiotech, Loos, France*

WP 062 **Isotyping Anti-Drug Antibodies using LC-MS/MS QTOF quantification of SIL peptides**; Cristian I. Ruse[1]; Ashish Vaswani[1]; Carl Luongo[1]; Hannah Zhang[1]; Srujan Gandham[1]; Matthew Digby[1]; Jason Delcarpini[1]; Darshana Jani[1]; Ling Morgan[1]; Serenus Hua[1]; *[1]Moderna Therapeutics, Cambridge, MA*

WP 064 **Online Enrichment of Low-Abundance Protein Biomarkers for Targeted LC-MS**; Nathaniel B. Axtell[1]; Thy Truong[1]; Alex Butters[1]; Jeffrey R. Whiteaker[2]; Lei Zhao[2]; Amanda G. Paulovich[2]; Ryan T. Kelly[1]; *[1]BYU, Provo, UT; [2]Fred 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; *National Taiwan Ocean University, Keelung, Taiwan*

WP 066 **Quantitative Analysis of Protein Ions Based in Isotopic Pattern Distortions**; Snehin R Momin[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

WP 067 **The Detection and Quantitation of Stercobilin in Autism Model Fecal Extracts Using LC-MS**; Erin R. Tiede[1]; Emily R. Sekera[2]; Troy D. Wood[1]; *[1]University at Buffalo, Buffalo, NY; [2]The Ohio State University, Columbus, OH*

WP 068 **timsTOF HT improves protein identification and quantitative reproducibility for deep unbiased plasma protein biomarker discovery**; Dijana Vitko[1]; Wan-Fang Chou[1]; Mark Marispini[1]; Sai Ramaswamy[1]; Sara Nouri Golmaei[1]; Yuntao Hu[1]; Joon Yong-Lee[1]; Megan Mora[1]; Jessica Chan[1]; Guillermo Flores-Campuzano[2]; John Blume[1]; Chinmay Belthangady[1]; Manway Liu[1]; Philip Ma[1]; Bruce Wilcox[1]; *[1]PrognomiQ, San Mateo, CA; [2]Switch 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 Needham[1]; Mitch Johnson[1]; Colt Cookson[1]; Joe Flynn[1]; Ron Bowsher[2]; Derrick Johnson[2]; Sanofar Jainul Abdeen[2]; Molly Madden[3]; Ben Barthel[3]; *[1]Veloxity Labs, LLC, Peoria, IL; [2]B2S Life Sciences, Franklin, IN; [3]Edgewise Therapeutics, Boulder, CO*

WP 071 **Mapping of the Human Cell Metabolome Identifies Novel Cancer Therapeutic Targets in MYC-amplified Group 3 Medulloblastoma**; William D Gwynne[1]; Yujin Suk[2]; Jeremy K Chan[1]; Stefan Custers[2]; Cunjie Zhang[1]; Andrew T Quaile[1]; Chitra Venugopal[2]; Sheila K. Singh[2]; Rafael Montenegro-Burke[1]; *[1]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; [2]Center for Discovery in Cancer Research, McMaster University, Hamilton, ON*

WP 072 **The Identification of the HLA Class I Immunopeptidome of Malignant Peripheral Nerve Sheath Tumors via Mass Spectrometry**; Kyle A Richards[1]; Suzanne Coleman[1]; Jessica Liebau[1]; Mitchell Hruska[1]; Tyler Jubenville[1, 2]; Reid Wagner[2]; Subina Mehta[3]; David A Largaespada[1, 2]; Timothy J Griffin[3]; *[1]Masonic Cancer Center, Department of Pediatrics, University of Minnesota, Minneapolis, MN; [2]Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN; [3]Biochemistry, Mol. Biology, and Biophysics, University of Minnestoa, Minneapolis, MN*

WP 073 **Detecting impending infections in immunocompromised cancer patients**; Sara Violante[1]; Ruben J. F. Ramos[1]; Hannah Lees[1]; Emma E. Rennie[2]; James S. Pyke[2]; Andrew D. McEachran[2]; Mark Sartain[2]; Justin R. Cross[1]; *[1]Memorial Sloan Kettering Cancer Center, New York, NY; [2]Agilent Technologies, Santa Clara, CA*

WP 074 **Multiomics approach to elucidate the role of endoplasmic reticulum-mitochondria contact sites in tumor metabolic rewiring**; Brandon Chen[1]; Pietro Morlacchi[2]; Costas Lyssiotis[1]; Yatrik Shah[1]; *[1]University of Michigan-Ann Arbor, Ann Arbor, MI; [2]Agilent Technologies, Lexington, MA*

WP 075 **Targeted proteomics for discovery of novel biomarkers in human plasma for early breast cancer diagnosis**; Margret Thorsteinsdottir[1]; Kristrun Yr Holm[1]; Kari Arnarsson[1]; Finnur Eiriksson[1]; Sigridur Klara Bodvarsdottir[2]; Yassene Mohammed[3]; Christoph H. Borchers[4]; *[1]Faculty of Pharmaceutical Sciences, University of Iceland, Reykjavik, Iceland; [2]BioMedical Center, University of Iceland, Reykjavik, Iceland; [3]Leiden University Medical Center, Leiden, Netherlands; [4]Segal 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 Wang[1]; Feng Wang[1]; Shan Li[1]; Chai Foong Lai[1]; Tsui-Fen Chou[1]; *[1]California 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 Wang[1]; Hongming Song[1]; Li Wang[1]; Santosh Renuse[2]; Kiran Mangalaparthi[1]; Akhilesh Pandey[1]; Xinyan Wu[1]; *[1]Mayo Clinic, Rochester, MN; [2]Thermo 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 Bench[1]; Manoj Kumar[1]; Daniel E Frigo[2]; Thomas L Pulliam[2]; Livia S. Eberlin[1]; *[1]Department of Surgery, Baylor College of Medicine, Houston, Texas; [2]Department 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]; *[1]Lester and Sue Smith Breast Center, Baylor College of Medicine, Houston, TX; [2]Department of Molecular and Human Genetics, Baylor College of Medicine, Houston, TX*

WP 080 **Comparative Proteomics studies of mono and co-cultured drug-resistant and -sensitive cancer cells**

reveal potential interaction targets; Zongkai Peng[1]; Zhibo Yang[1]; Ahsan Nagib[1, 2]; *[1]University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; [2]Mass 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 Banerjee[1]; Sanjeeva Srivastava[1]; *[1]IIT Bombay, Mumbai, India*

WP 082 **Role of MGAT3 and "Bisecting GlcNAc" N-glycans in TGF-β1 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 Cheng[1]; Pietro Morlacchi[2]; Li Zhang[3]; Pete Sajjakulnkit[4]; Jasmine Wisniewski[5]; Bailey Jackson[5]; Yuanyuan Qiao[6]; Costas Lyssiotis[7]; Arul M Chinnaiyan[6]; *[1]Graduate Program in Cell and Molecular Biology, University of Michigan, Ann Arbor, Michigan; [2]Agilent Technologies, Lexington, MA; [3]School of Medicine, University of Michigan, Ann Arbor, Michigan; [4]Doctoral Program In Cancer Biology, University of Michigan, Ann Arbor, Michigan; [5]College of LSA, University of Michigan, Ann Arbor, Michigan; [6]Michigan Center for Translational Pathology, Department of Pathology, University of Michigan, Ann Arbor, Michigan; [7]Department 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 Stolley[1]; Maria Sophia Stenkamp[1]; Natalie Fowlkes[1]; Erin H Seeley[2]; Erik Cressman[1]; *[1]MD Anderson Cancer Center, Houston, TX; [2]University 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 Joseph[1]; Nicolas Leon Young[2, 3]; *[1]baylor college of medicine, houston, TX; [2]Verna & Marrs McLean Department of Biochemistry & Molecular Biology, Baylor College of Medicine, Houston, TX; [3]Department 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 Molina[1]; Pietro Morlacchi[2]; Jefferey Song[1]; Sonal Gera[1]; *[1]Ribon Therapeutics, Cambridge, Massachusetts; [2]Agilent 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 Letelier[1]; Ali Hussein Abdel Sater[1]; Yihui Chen[1]; Ranran Wu[1]; Jennifer B Dennison[1]; Soyoung Park[1]; Ehsan Irajizad[1]; Hiroyuki Katayama[1]; Jody Vykoukal[1]; Samir M Hanash[1]; Edwin J Ostrin[1]; Johannes Fahrmann[1]; *[1]MD 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 Lum[1]; Oscar Pundel[2]; William A Hofstadter[1]; John Muroski[1]; Benjamin G Neel[2]; Ileana M Cristea[1]; *[1]Princeton University, Princeton, NJ; [2]NYU Langone Health, New York, NY*

WP 089 **Regulation of the FKBP10 transcriptional locus in lung metastasis**; Bryan Rivas[1]; Alexander B. Saltzman[1]; Doug Chan[2]; Anna Malovannaya[1]; *[1]Baylor College of Medicine, Houston, Texas; [2]MD Anderson, Houston, TX*

WP 090 **Proteomics investigation of gliomas resected after 5-ALA fluorescence guided surgery reveals molecular heterogeneity driving differential fluorescence**; Saicharan Ghantasala[1]; Amruth Bhat[2]; Aliasgar Moiyadi[3, 4]; Sridhar Epari[3, 4]; Sanjeeva Srivastava[5]; *[1]Centre for Research in Nano Technology and Science, Indian Institute of Technology Bombay, Mumbai, India; [2]Centre for BioSystems Science and Engineering, Indian Institute of Science, Bengaluru, India; [3]Department of Neurosurgery, Tata Memorial Centre's – Advanced Centre for Treatment, Research and Education in Cancer, Navi Mumbai, India; [4]Homi Bhabha National Institute, Mumbai, India; [5]Deparment 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 Singh[1]; Zongkai Peng[1]; Zhibo Yang[1]; Anthony Burgett[2]; *[1]University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK; [2]The 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 Fariha[1]; Zahra Ahmed[1]; Jad Hamze[1]; Emma Rothkopf[1]; Oluwanifemi Okoh[1]; Anubhav Tripathi[1]; *[1]Brown University, Providence, RI*

WP 093 **Identification of metabolic pathways driven by SMARCB1 deficiency in bladder cancer**; Chandra Sekhar Amara[1]; Abu Hena Mostafa Kamal[1]; Danthasinghe Waduge Badrajee Piyarathna[1]; Arun Sreekumar[1]; Msaouel Pavlos[2]; Nagireddy Putluri[1]; *[1]Baylor College of Medicine, Houston, Texas; [2]MD Anderson, Houston, TX*

WP 094 **Identification of altered mitochondrial metabolism in bladder cancer disparity**; Karthik Reddy Kami Reddy[1]; Junhyoung Park[1]; Vasanta Putluri[1]; Danthasinghe Waduge Badrajee Piyarathna[1]; Martha K Terris[2]; Seth P Lerner[1]; Yair Lotan[3]; Benny Abraham Kaipparettu[1]; Nagireddy Putluri[1]; *[1]Baylor College of Medicine, Houston, TX; [2]Augusta university, Augusta, Georgia; [3]UT Southwestern Medical Center, dallas, Texas*

WP 095 **LC-MS method to measure the D- and L-2-Hydroxyglutarate in Cerebrospinal Fluid**; Satwikreddy Putluri[1]; Abu Hena Mostafa Kamal[2]; Leomar Y Ballester[3]; *[1]University of Texas MD Anderson Cancer Center, Houston, TX; [2]Baylor College of Medicine, Houston, Texas; [3]MD Anderson, Houston, TX*

WP 096 **Application of the MasSpec Pen Technology for Molecular Identification of Human Sarcomas and Surgical Margin Evaluation**; Ashley E. Montgomery[1]; Justin E. Bird[2]; Douglas Fletcher[2]; Sharon Landers[3]; Sintawat Wangsiricharoen[4]; Wei-Lien Wang[4]; Wendong Yu[4]; Livia S. Eberlin[5]; Keila E. Torres[3]; *[1]Baylor College of Medicine, Department of Student Affairs, Houston, Texas; [2]MD Anderson Cancer Center, Division of Surgery, Department of Orthopedics, Houston, Texas; [3]MD Anderson Cancer Center, Division of Surgery, Department of Surgical Oncology, Houston, Texas; [4]MD Anderson Cancer Center, Division of Pathology Lab-Medicine, Department of Pathology, Houston, Texas; [5]Baylor 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 Kim[1]; Neil G. Patel[1, 2]; Ryan Joseph Weiss[1, 2]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]Complex Carbohydrate Research Center, Athens, GA*

WP 098 **Does The Chemistry of Glycosidic Bond Cleavage Vary?**; Joy Namachanja Malaba[1]; Lauren Schultz[1]; Lauren Davis[1]; Dylan Carter[2]; Benjamin Bythell[2]; *[1]Ohio University, Athens, OH; [2]Ohio University, Athens, OH*

WP 099 **Combined Tandem Mass Spectrometry and Computational Chemistry for Structural Elucidation of Singly and Doubly Deprotonated Galacturonic Acids**; Ola Bataineh[1]; Jordan Rabus[1]; Rebecca Flinchbaugh[1]; Dylan Carter[1]; Lauren Davis[1]; Benjamin Bythell[1]; *[1]Ohio University, Athens, OH*

WP 100 **N-Glycan Quantitation andCharacterizationvia HILIC-FLD-ESI/MS Using a Novel Fluorescence Free RadicalReagent**; Shane Finn[1]; Rayan Murtada[1]; Wilthon Gilles[1]; Jinshan Gao[1]; *[1]Montclair State University, Montclair, NJ*

WP 101 **Mass Spectrometry-based High-throughput Profiling of Porcine Notochordal-Cell MatrixN-glycans Using GlycanExplorer™ Software**; Rupanjan Goswami[1]; Kieran Joyce[2]; Büşra Günay[2]; Melanie Ng Tung Hing[3, 4]; Caitriona Walsh[5]; Tara Schmitz[6]; Marianna Tryfonidou[7]; Keita Ito[6]; Karthik Kolli[1]; Abhay Pandit[2]; Radka Saldova[2, 3, 4]; Arun Apte[1]; *[1]PREMIER Biosoft, San Francisco, CA; [2]CÚRAM, SFI Research Centre for Medical Devices, National University of Ireland, Galway, Galway, Ireland; [3]GlycoScience group, National Institute for Bioprocessing Research and Training (NIBRT), Dublin, Ireland; [4]UCD School of Medicine, College of Health and Agricultural Science, University College Dublin, Dublin, Ireland; [5]Contract Research group, National Institute for Bioprocessing Research and Training (NIBRT), Dublin, Dublin, Ireland; [6]Orthopaedic Biomechanics, Department of Biomedical Engineering, Eindhoven University of Technology, Eindhoven, Eindhoven, Netherlands; [7]Department 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 Choi[1]; I. Jonathan Amster[1]; Jandi Kim[1]; *[1]University of Georgia, Athens, GA*

WP 103 **Characterizing degradation products from Bacteroides thetaiotaomicron to understand bacterial dextran utilization in the gut**; Neil Gregory Rumachik[1]; Tian Tian[1]; Hannah Gibson[2]; David Bolam[2]; Yan Liu[1]; Fiona Cuskin[2]; *[1]Thermo Fisher Scientific, Sunnyvale, CA; [2]Newcastle 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 Roberts[1]; Jandi Kim[1]; Stephanie Archer-Haartman[1, 2]; Lachlan James Smith[3]; Jonathan Amster[1]; Zhirui Jiang[4]; Yian Khai Lau[3]; Margaret Casal[3, 5]; *[1]University of Georgia, Athens, GA; [2]Complex Carbohydrate Research Center, Athens, GA; [3]University of Pennsylvania, Philadelphia, PA; [4]Forsyth Institute, Cambridge, Massachusetts; [5]University of Pennsylvania School of Veterinary Medicine, Philladelphia, Pennsylvania*

WP 105 **Isomeric Separation of Permethylated Glycans using LC-FAIMS-MS/MS**; Md Abdul Hakim[1]; Akeem Adeyemi Sanni[1]; Waziha Purba[1]; Oluwatosin Daramola[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 106 **Isomeric separation of native N-glycans using nano ZIC-HILIC column**; Oluwatosin E Daramola[1]; Cristian D Gutierrez-Reyes[1]; Judith Nwaiwu[1]; Mojibola Fowowe[1]; Sherifdeen Onigbinde[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 107 **HCD, ETD, and EThcD Fragmentation Spectra of Co2+-Adducted Human Milk Oligosaccharides Distinguish Linkage Isomers**; Sebastian N Alberti[1]; Darren Gass[1]; Elyssia S. Gallagher[1]; *[1]Baylor 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]; *[1]Graduate School of Analytical Science and Technology, Chungnam National University, South Korea; [2]Asia-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 Termoul[1]; Stéphanie Flament[1]; Fabrice Bray[1]; Christian Rolando[1, 3]; *[1]UAR CNRS 3290 - MSAP, Villeneuve d'ascq, France; [2]Lesaffre International - R&D analytical department, Marquette-Lez-Lille, France; [3]Shrieking Sixties - 1-3 Allée Lavoisier, Villenueve d'Ascq, France*

WP 110 **Structural and compositional characterization of dissolved hemicellulose with 12-T ESI FT-ICR in positive and negative ion modes**; Mikko Nikunen[1]; Timo Kekäläinen[1]; Janne Jänis[1]; *[1]University of Eastern Finland, Department of Chemistry, Joensuu, Finland*

WP 111 **Sensitive Analysis and Differentiation of Oligosaccharides Isomers by Direct Infusion Mass Spectrometry**; Enoch Amoah[1]; Abraham Kwame Badu-Tawiah[2]; *[1]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; [2]The Ohio State University, Columbus, OH*

WP 112 **Developing Novel capillary electrophoresis tandem mass spectrometry strategies for the characterization of complex mixture Heparan sulfates**; Yiqing Zhang[1]; Jonathan Amster[2]; *[1]University of Georgia, Department of Chemistry, Athens, GA; [2]University of Georgia, Athens, GA*

WP 113 **Optimization of PRM-LCMS/MS for Glycosaminoglycan Disaccharide Profiling in C. Elegans**; Lauren Heidenreich[1]; Franklin E. Leach III[1]; *[1]University 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 Li[1]; Yu-Shing Cheng[1]; *[1]Institute 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. Mishra[1]; William G. Gutheil[1]; *[1]University 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 Oakley[3]; Jennifer J Couper[3]; Leonard C Harrison[2, 4]; John M Wentworth[2, 4]; Toby Dite[1, 2]; Andrew I Webb[2, 5]; Laura F Dagley[1, 2]; *[1]Advanced Technology and Biology Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Melbourne, Australia; [2]Department of Medical Biology, University of Melbourne, Parkville, Melbourne, Australia; [3]Faculty of Faculty Health and Medical Sciences, The University of Adelaide, Adelaide, Australia; [4]Population Health Division, The Walter and Eliza Hall Institute of Medical Research, Parkville, Melbourne, Australia; [5]Colonial 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 Guzman[1]; Ana Martinez Del Val[1]; Zilu Ye[1]; Florian Harking[1]; Tabiwang N. Arrey[2]; Anna Pashkova[2]; Hamish Stewart[2]; Yue Xuan[2]; Nicolaie Eugen Damoc[2]; Jesper V. Olsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; [2]Thermo 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 Furrer[2]; Alexander Schmidt[1, 2]; *[1]Proteomics Core Facility, University of Basel, Basel, Switzerland; [2]Biozentrum, 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 Distler[1]; Mateusz Krzysztof Łącki[1]; Michał

Piotr Startek[1]; David Teschner[2]; Sven Brehmer[3]; Jens Decker[3]; Thilo Schild[1]; Jonathan Krieger[4]; Florian Krohs[3]; Oliver Raether[3]; Andreas Hildebrandt[2]; Stefan Tenzer[1, 5]; [1]*Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany;* [2]*Institute for Informatics, Johannes-Gutenberg University Mainz, Mainz, Germany;* [3]*Bruker Daltonics GmbH & Co.KG, Bremen, Germany;* [4]*Bruker Ltd, Milton, ON;* [5]*Helmholtz Institute for Translational Oncology (HI-TRON), Mainz, Germany*

WP 120 **Benchmarking commonly used software suites and analysis workflows for DIA proteomics and phosphoproteomics**; Ronghui Lou[1]; Ye Cao[2]; Shanshan Li[1]; Yaoyang Zhang[2]; Wenqing Shui[1]; [1]*ShanghaiTech University, Shanghai, China;* [2]*Chinese Academy of Sciences, Shanghai, China*

WP 121 **Cross-lab Evaluation of Quality Control for Large-scale Data-Independent Acquisition-based quantitative proteomics**; Gaohuanhuan Gao[1]; He Wang[1]; Yantao Li[2]; Zhongxiang Ni[2]; Yi Zhu[1]; Tianan Guo[1]; [1]*Westlake University, Hangzhou, China;* [2]*WestLake 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 Skowronek[1]; Georg Wallmann[1]; Maria Wahle[1]; Ericka C. M. Itang[1]; Polina Koval[1]; Marvin Thielert[1]; Florian Krohs[2]; Markus Lubeck[2]; Sander Willems[3]; Oliver Raether[2]; Matthias Mann[1, 4]; [1]*Max Planck Institute of Biochemistry, Martinsried, Germany;* [2]*Bruker Daltonics GmbH & Co.KG, Bremen, Germany;* [3]*Bruker Belgium nv, Kontich, Belgium;* [4]*Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark*

WP 123 **Multiplexed data-independent acquisition (DIA) using a novel high-resolution accurate mass spectrometer**; Sophia Steigerwald[1]; Wen-Feng Zeng[1]; Maximilian T. Strauss[2]; Marvin Thielert[1]; Ulises H. Guzmán[2]; Nicolaie Eugen Damoc[3]; Stevan Horning[3]; Jesper V. Olsen[2]; Matthias Mann[1, 2]; [1]*Max Planck Institute of Biochemistry, Martinsried, Germany;* [2]*Novo Nordisk Foundation Center for Protein Research, University of Copenhagen, København, Denmark;* [3]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

WP 124 **Single-Shot deep DIA LCMS workflow for near-full proteome coverage**; Robert Van Ling[1]; Amirmansoor Hakimi[2]; Santosh Renuse[2]; Paul Jacobs[3]; Jeff Op De Beeck[3]; [1]*Thermo Fisher Scientific, Breda, Netherlands;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*Thermo 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 Krieger[1]; Patrick Von Zalm[2]; Arthur Viode[2]; Hanno Steen[2, 3]; Judith Steen[4]; [1]*Bruker Ltd., Milton, ON;* [2]*Department of Pathology, Boston Children's Hospital, Harvard Medical School, Boston, MA;* [3]*Neurobiology Program and Precision Vaccines Program, Boston Children's Hospital, Boston, MA;* [4]*Neurobiology 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 Robinson[1]; Yuchen He[2]; Evgenia Shishkova[2]; Katherine A Overmyer[2, 3]; Joshua J. Coon[2, 3]; [1]*University of Wisconsin, Madison, Madison, WI;* [2]*University of Wisconsin-Madison, Madison, WI;* [3]*Morgridge Institute for Research, Madison, WI*

WP 127 **Deciphering the molecular pathway driving cell competition using DIA label-free mass spectrometry**; Suniya Khatun[1]; Riccardo Zenezini Chiozzi[1, 2]; Manasi Kelker[3]; Guillaume Charras[3, 4, 5]; Alan Lowe[1, 3, 4, 6]; Konstantinos Thalassinos[1, 2, 7]; [1]*Department of Structural and Molecular Biology - UCL, London, United Kingdom;* [2]*Mass Spectrometry Science Technology Platform - UCL, London, United Kingdom;* [3]*London Centre for Nanotechnology - UCL, London, United Kingdom;* [4]*Institute for the Physics of Living Systems - UCL, London, United Kingdom;* [5]*Department of Cell and Developmental Biology - UCL, London, United Kingdom;* [6]*The Alan Turing Institute, London, United Kingdom;* [7]*Institute 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 Muroski[1]; Gabriel Navarro[1]; Mona Elbadawi[1]; [1]*Amyris, Emeryville*

WP 129 **Optimizing dia-PASEF isolation window schemes for proteomics measurements on a timsTOF instrument**; Markus Lubeck[1]; Stephanie Kaspar-Schoenefeld[1]; Christoph Krisp[1]; Andreas Schmidt[1]; Florian Busch[1]; Eduardo Carrascosa[1]; Oliver Raether[1]; Gary Kruppa[2]; [1]*Bruker Daltonics GmbH & Co. KG, Bremen, Germany;* [2]*Bruker S.R.O., Brno, Czech Republic*

WP 130 **Integrating permethylation and Zeno SWATH method to characterize nucleic acid modifications**; Yixuan (axe) Xie[1]; Ye Chen[1]; Francisca N De Luna Vitorino[1]; Zongtao Lin[1]; Xingyu Liu[1]; Emily Zahn[1]; Arabella Garcia[1]; Benjamin A. Garcia[1]; [1]*Washington 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. Akinlaja[1]; Brenna H. Hay[1]; Teesha C. Baker[1]; Aicha A. Houfani[1]; Greg R. Stacey[1]; Leonard J. Foster[1]; [1]*University of British Columbia, Vancouver, BC*

WP 132 **Data-Independent Analysis of Human Eye Lens Proteome Reveals New Sites of Aspartic Acid Isomerization**; Evan E Hubbard[1]; Yana Lyon[2, 3]; Ryan R. Julian[1]; [1]*University of California, Riverside, Riverside, CA;* [2]*Inhibrx Inc., La Jolla, 92037;* [3]*University 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. Midha[1]; Charu Kapil[1]; Michal Maes[1]; David H. Baxter[1]; Seamus R. Morrone[1]; Timothy J. Prokop[1]; Robert L. Moritz[1]; [1]*Institute 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 Bandyopadhyay[1]; Erin D. Jeffery[1]; Qing Yu[2]; Ben Jordan[3]; Gloria Sheynkman[1, 4, 5, 6]; [1]*Department of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville, Virginia, USA, Charlottesville, VA;* [2]*Department of Cell Biology, Harvard Medical School, Boston, MA, USA, Boston, MA;* [3]*Cancer Genomics Research Laboratory, Frederick National Laboratory for Cancer Research, Frederick, MS USA, Frederick, MD;* [4]*Department of Biochemistry and Molecular Genetics, University of Virginia, Charlottesville, VA, USA, Charlottesville, VA;* [5]*Center for Public Health Genomics, University of Virginia, Charlottesville, VA, USA, Charlottesville, VA;* [6]*UVA 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 Distler[1]; Mateusz Krzysztof Łącki[1]; Michał Piotr Startek[2]; David Teschner[3]; Jonathan Krieger[4]; Florian Krohs[5]; Oliver Raether[5]; Stefan Tenzer[1]; [1]*Institute for Immunology, University Medical Center of the Johannes-Gutenberg University Mainz, Mainz, Germany;* [2]*Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland;* [3]*Institute for Informatics,* *Johannes-Gutenberg University Mainz, Mainz, Germany; [4]Bruker Ltd, Milton, ON L9T 6P4; [5]Bruker 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 Plumb[1]; Andrew Leightner[1]; Ian D Wilson[2]; Billy J Molloy[3]; Russell Mortishire-Smith[3]; *[1]Waters, Milford, MA; [2]Imperial College, London, London, United Kingdom; [3]Waters Corporation, Wilmslow, United Kingdom*

WP 137 **Ultra-High Throughput Metabolic Stability Assay using Acoustic Ejection Mass Spectrometry**; Jacob Watson McCabe[1]; Anuja Bhalkikar[1]; Han Joo Lee[1]; *[1]SCIEX, Frammingham, MA*

WP 138 **Assessment of Chromatographic Performance in High-Throughput ADME Screening**; Carson Powell[1]; John Janiszewski[1]; Ross Wallace[1]; *[1]Loxo 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 Yoo[1]; *[1]Hanyang University, Ansan, South Korea; [2]Brigham 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 Rizi[1]; Rahul Baghla[2]; Eshani Nandita[2]; *[1]Sciex, Framingham, MA; [2]SCIEX, 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 Jiang[1]; Phuong Nguyen[1]; Quanyun Alan Xu[1]; Qi Wu[1]; Thomas Quill[1]; *[1]University of Texas MD Anderson Cancer Center, Houston, TX*

WP 142 **Metabolite profiling and characterization byion mobility LC-timsTOF Pro PASEF**; Xuejun Peng[1]; Surendar Tadi[2]; Beixi Wang[1]; Erica Forsberg[1]; *[1]Bruker Daltonics Inc., San Jose, CA; [2]Bruker 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. Rehm[1]; Birju Patel[1]; Mitchell J. Martineau[1]; Shantanu Roychowdhury[1]; *[1]Eurofins Panlabs, Saint Charles, MO*

WP 144 **Global profiling of AMG510 modified proteins identified tumor suppressor KEAP1 as an off-target**; Yini Wang[1]; Bowen Zhong[2]; Caixia Xu[2]; Dongdong Zhan[2]; Yi Wang[2]; Jun Qin[2]; *[1]National Center for Protein Sciences (The PHOENIX Center, Beijing), Beijing, China; [2]National Center for Protein Sciences (The PHOENIX Center, Beijing), Beijing, China*

WP 145 **LC-MS metabolic profiling of a standardized extract of PACs fromVitis viniferaseeds in healthy volunteers andin-vitrosupporting studies**; Giovanna Baron[1]; Larissa Della Vedova[1]; Francesca Gado[1]; Laura Fumagalli[1]; Marina Carini[1]; Cristian Del Bo[2]; Paolo Morazzoni[3]; Giancarlo Aldini[1]; *[1]Department of Pharmaceutical Sciences (DISFARM), Università degli Studi di Milano, Milan, Italy; [2]Department of Food, Environmental and Nutritional Sciences, Università degli Studi di Milano, Milan, Italy; [3]Divisione Nutraceutica, Distillerie Umberto Bonollo S.p.A, Mestrino, Italy*

WP 146 **Determination of Bicalutamide in Human and Mouse serum using PerkinElmer QSight 420 LC-MS/MS system with Epic C18 column**; Sergey Shulga-Morskoy[1]; Cole Strattman[2]; *[1]Perkin Elmer Health Sciences Inc, Hopkinton, MA; [2]Perkin Elmer, shelton, CT*

WP 147 **Open Port Interface with Electromagnetic Mixing for an Affinity Selection MS System**; Thomas R. Covey[1]; Chang Liu[1]; Peter Kovarik[1]; Jonathan Shrimp[2]; Nate Hoxie[2]; Michael Ronzetti[2]; Bolormaa Baljinnyam[2]; Colin Kelly[2]; John Janiszewski[2]; Meghav Verma[2]; Sam Michael[2]; Matthew Hall[2]; Anton Simeonov[2]; Richard Van Breemen[3]; Yuandan Liu[4]; Jianli Zhao[4]; Emmet Welch[4]; *[1]SCIEX, Concord, ON; [2]National Center For Advancing Translational Sciences, Rockville, MD; [3]Oregon State University, Corvallis; [4]Phenomenex, Torrance, CA*

WP 148 **Microtiter well based MS method scheduling for high-throughput mass spectrometry**; David Cox[1]; Chang Liu[1]; Bogdan Georgescu[1]; *[1]SCIEX, 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 Athanason[1]; Sheri Smith[1]; Bennett Ma[1]; Karsten Menzel[1]; *[1]Pharmacokinetics, 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 Mendoza[1]; Mark Athanason[1]; Michelle Robinson[1]; Xiaoyan Chu[1]; Jingjing Guo[1]; Matthew Mazur[1]; Weixun Wang[1]; *[1]Merck & Co., Inc., West Point, PA*

WP 151 **Mitragynine UPLC-MS/MS Method Development and Preclinical Pharmacokinetics**; China Ryu[1]; Natalie R. Hagen[1]; Junfeng Huang[1]; Xin Xu[1]; Amy Q. Wang[1]; *[1]National 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 Spencer[1]; Malcolm R. Clench[1]; Vikki Carolan[1]; Stephen Rumbelow[2]; *[1]BMRC, Sheffield Hallam University, Sheffield, United Kingdom; [2]CRODA 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. Siegel[1]; Gary E Walker[1]; Serhiy Hnatyshyn[2]; *[1]MS Mass Spec Consultants, Fair Lawn, NJ; [2]BMS, 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 Chen[1]; Jingduan Chi[2]; Melissa Mofikoya[2]; Lei Shi[1]; *[1]Sunovion Pharmaceuticals Inc., Marlborough, MA; [2]PPD, Middleton, WI*

WP 155 **Quantification of Sazetidine-A from Rat Brain and Plasma for the Treatment of Tinnitus**; Emily M Hubecky[1]; Samantha A Olendorff[2]; Donald Caspary[3]; Lynne Ling[3]; Kevin R Tucker[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, Illinois; [2]Shimadzu, Columbia, MD; [3]Southern 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 Chi[1]; Melissa Mofikoya[1]; Zhijing Huang[1]; *[1]PPD 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 Pan[1]; Chia-Fang Wu[1, 2]; Ming-Tsang Wu[3, 4, 5, 6]; *[1]Kaohsiung Medical University Research Center for Environmental Medicine, Kaohsiung city, Taiwan; [2]International Master Program of Translational Medicine, National United University, Miaoli city, Taiwan; [3]Kaohsiung Medical University Research Center for Environmental Medicine, Kaohsiung city, Taiwan; [4]Ph.D. Program in Environmental and Occupational Medicine, College of Medicine, Kaohsiung Medical University, Kaohsiung city, Taiwan; [5]Department of Public Health, College of Health Sciences, Kaohsiung Medical University, Kaohsiung city, Taiwan; [6]Department 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

Jianli[1]; Li Qiang[2]; Hao Hongyuan[2]; *[1]Shimadzu (China) Co., Ltd.,, Wuhan, China; [2]Shimadzu(China)Co.,LTd, Shanghai, China*

WP 159 **Structure elucidation of a macrocyclic GSH-adduct metabolite of Rilzabrutinib, a reversible covalent BTK inhibitor**; Cathy Muste[1]; Shu-Yu Liao[1]; Chungang Gu[1]; *[1]Biogen, Cambridge, MA*

WP 160 **Novel Application of LC-MS to Qualitatively Identify Underivatized Metoprolol Acid in Equine Plasma to Prove Metoprolol Administration**; Benjamin J Burris[1]; Halie A Copley[1]; Mark A Musetti[1]; Deidre E Damon[1]; Ryan M Farmer[1]; Soobeng Tan[1]; *[1]Ohio Department of Agriculture, Reynoldsburg, OH*

WP 161 **Exploring the Applicability of Multi-Reflecting Time-of-Flight Mass Spectrometry for Expedited Biotransformation Studies**; Daniel J Weston[1]; Emma Marsden-Edwards[2]; Martin Palmer[2]; Laura Tomlinson[1]; Richard Gregory[1]; Kevin Colizza[3]; Alexandr Muck[4]; *[1]GSK, Stevenage, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom; [3]GSK, Collegeville, PA; [4]Waters Corporation, Wilmslow, United Kingdom*

WP 162 **Pharmacokinetics of Ketamine Transfer into Human Milk**; Palika Datta[1]; Kaytlin Krutsch[1]; Teresa Baker[1]; Thomas Hale[1]; *[1]Texas Tech University Health Sciences Center, Amarilo, TX*

WP 163 **Mass spectrometry analysis of the contradiction between antiparasitic protection and immune responses in a Chagas disease nonhuman primate vaccination model**; Zongyuan Liu[1]; Priscila Silva Grijó Farani[2]; John L. Vandeberg[3]; Igor C. Almeida[2]; Laura-Isobel McCall[1]; *[1]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK; [2]Border Biomedical Research Center, University of Texas El Paso, El Paso, TX; [3]Department 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 Nguyen[1]; Ryan P Seguin[1]; Libin Xu[1]; *[1]University of Washington, Seattle, WA*

WP 165 **Multi-Elemental Detection of Heteroatoms for Standard-Free Quantitation of Xenobiotics**; Grace E Hahm[1]; Frenio A Redeker[1]; Kaveh Jorabchi[1]; *[1]Georgetown 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 Zarrouk[1]; Alan Barnes[2]; Stephane Moreau[3]; Neil Loftus[2]; Sylvain Dulaurent[1]; Souleiman Elbalkhi[1]; Franck Saint-Marcoux[1]; *[1]CHU Limoges, Limoges, France; [2]Shimadzu Corporation, Manchester, United Kingdom; [3]Shimadzu 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 Schwemler[1]; Hoora Shaghaghi[1]; *[1]Alliance Pharma Inc, Malvern, PA*

WP 168 **Improved Quantitation of Sulfated Compounds in Human Plasma and Urine through Hydrolysis with Purified Arylsulfatase**; Amanda C. McGee[1]; Douglas Waites[1]; L. Andrew Lee[1]; *[1]Integrated 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 Johnson[1]; Xiaorong Liang[1]; Brian Dean[1]; Shuguang Ma[1]; Sungjoon Cho[1]; *[1]Genentech 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 Fincher[1]; Ismael Zamora[2]; Mark Cancilla[1]; *[1]Merck & Co., West Point, PA; [2]Lead 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 Alsibaee[1]; Ali S Abdelhameed[1]; Mohamed W. Attwa[1]; Adnan A Kadi[1]; *[1]College 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 Aljohari[1]; Adham Bahian[1]; Adnan A Kadi[1]; A. F. M. Motiur Rahman[1]; *[1]King Saud University, Riyadh, Saudi Arabia*

WP 173 **Polymer StudioTM: a novel software for fast profiling and identifying complex pharmaceutic excipients by UHPLC-HRMS/MSntechnique**; Zhe Wang[1]; Jiamin Gao[2]; Xinjian Li[1]; Yanan Wang[1]; Ning Sheng[1]; Runtao Tian[2]; Jinlan Zhang[1]; *[1]Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing, China; [2]Chemmind 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 Duchoslav[1]; Harini Kaluarachchi[1]; Giulia Calloni[2]; *[1]SCIEX, Concord, ON; [2]SCIEX, 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 Stevens[1]; Lindsay Hatch[1]; Sarah Dowd[1]; Frank Dorman[1]; *[1]Waters, Milford, MA*

WP 176 **A Quick MRM Method for FASAs Analysis in Surface Water Using UHPLC-MS/MS**; Danyang Wang[1]; Vanisree Mulabagal[1]; Meredith Feltman[1]; Roger Viticoski[1]; Joel Hayworth[1]; *[1]Auburn 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 Sanchez[1]; Ralf Tautenhahn[2]; *[1]ThermoFisher Scientific, Redwood City, CA; [2]ThermoFisher Scientific, San Jose, CA*

WP 178 **Total Fluorine Quantitation by Plasma Assisted Reaction Chemical Ionization Mass Spectrometry**; Samuel R White[1]; Kaveh Jorabchi[1]; *[1]Georgetown 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. Granger[1]; Heather A. Brant[1]; Haley B. Lawton[1]; Stephanie N. Gamble[1]; Amie C. McElroy[1]; Joseph M. Mannion[1]; *[1]Savannah 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 Camacho[1]; John A. Bowden[1]; *[1]University 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 Robbins[1]; Deisy Giraldo[4]; Joseph Frye-Jones[2]; Chad Weisbord[1]; Alan G Marshall[1, 2]; Brice Bouyssiere[4, 5]; Pierre Giusti[5, 6]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; [3]International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harfleur, France; [4]Université de Pau et des Pays de l'Adour, Pau, France; [5]International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harfleur, France; [6]TotalEnergies OneTech R&D, TotalEnergies Research & Technology, Gonfreville, France*

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 Elliott[1]; Hussain A Abdulla[1]; [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 Fornadel[1]; Tomoko Vincent[2]; Dhinesh Asogan[2]; Daniel Kutscher[2]; Jon Peters[3]; Matthew Cassap[4]; [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 Mazur[1]; Sergey Sypalov[2]; Il'ya Varsegov[2]; Artiom Surmillo[1]; Nikolay V Ul'anovskii[2]; Dmitry S. Kosyakov[2]; Albert T Lebedev[1]; [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. Abubaker[1]; Jim H Scrivens[1]; Chris Ennis[1]; Jackie A Mosely[2]; [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 Baesu[1]; Yong-Lai Feng[1]; [1]*Health Canada, Ottawa, ON*

WP 190 **UV-induced photodegradation of emerging para-phenylenediamine quinones in aqueous environment**; Wei Wang[1]; Guodong Cao[1]; Jing Zhang[1]; Han Qiao[1]; Huankai Li[1]; Yanyan Chen[1]; Yuecheng Sang[1]; Zongwei Cai[1]; [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 Mathai[1]; Shailesh Sadashiv Damale[1]; Atul Narkar[1]; Kumar Raju[1]; Rajendra Makhamale[1]; [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. Selby[1]; Gabriel A. Bressendorff[1]; Lauren H. Phan[1]; Noah E. Hanratty[1]; Sydney R. Worth[1]; Tyson A. Lobb[1]; Hannah A. Konschak[1]; Claire E. Korte[1]; Carolyn J. Butts-Wilmsmeyer[1]; Kevin R. Tucker[1]; [1]*Southern Illinois University Edwardsville, Edwardsville, IL*

WP 193 **Real-Time Monitoring of PFAS in Air with PTR-MS**; Christian Lindinger[1]; Alfons Jordan[1]; Tobias Reinecke[1]; Rene Gutmann[1]; Andreas Mauracher[1]; Jens Herbig[1]; Lukas Märk[1]; Todd Rogers[2]; Philipp Sulzer[1]; [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 Carrascal[1]; Mira Čelić[2, 3]; Ester Sánchez-Jiménez[1]; Antoni Ginebreda[4]; Joaquin Abian[1]; Mira Petrovic[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 Heuvel[1]; Johan Scholtens[1]; Tamara Haagsma[1]; Stephane Moreau[2]; [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 Rochon[1]; Serge Auger[1]; Jean Lacoursière[1]; Pierre Picard[1]; [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 Martens[1]; Hendryk Czech[1]; Olli Sippulla[2]; Sven Ehlert[3]; Andreas Walte[3]; Ralf Zimmermann[1]; [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 Curtis[1]; David A Weil[2]; [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 Lock[1]; Rachel J Sanig[2]; Sarah Dowd[3]; Lee Gethings[4]; Nick Morley[5]; [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 Weil[1]; Andrew McEachran[1]; Cate Simmermaker[1]; Sarah Stow[1]; [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-Manso[1]; Tytus D. Mak[1]; Edward Erisman[1]; Kelly H. Telu[1]; Xiaoyu Yang[1]; Yuxue Liang[1]; William E. Wallace[1]; Stephen E. Stein[1]; [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-Fulmer[1]; David E Alonso[1]; Joseph E Binkley[1]; [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 Cardin[1]; Weier Hao[1]; John Quintana[1]; [1]*Entech Instruments, Simi Valley, CA*

WP 205 **High-Throughput Characterization of Fentanyl Analogs using LC-TIMS-TOF MS/MS**; Andrew R Forero[1]; Lilian Valadares Tose[1]; Matthew Willetts[2]; Melvin A. Park[2]; 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*

WP 206 **Combining DART-MS and GC-EI-MS Spectral Signatures for Classifying an Unknown Seized Drug: An Exploratory Approach**; William J Feeney[1]; Edward Sisco[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

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 Banidol[1]; Sophia Kouider[2]; Hélène Pizzala[2]; Laurence Charles[2]; *[1]Aix Marseille Université, CNRS, Institut de Chimie Radicalaire, MARSEILLE, France; [2]Aix Marseille Université, 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. Bain[1]; Patrick W. Fedick[2]; Tj Pinedo; Christopher C. Mulligan[3]; Shane Kullen[1]; Gui-hua Lang[1]; Douglas J. Klapec[1]; *[1]Bureau of Alcohol, Tobacco, Firearms and Explosives, Beltsville, MD; [2]Naval Air Warfare Center, United States Navy Naval Air Systems Command (NAVAIR), China Lake, CA; [3]Illinois 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 Prunty[1]; Nicholas Manicke[2]; Elizabeth Dhummakupt[3]; Dan Carmany[4]; *[1]Indiana University-Purdue University Indianapolis, Indianapolis, IN; [2]Indiana University Purdue University Indianapolis, Indianapolis, IN; [3]U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; [4]EXCET 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 West[1]; Michael G Leeming[1]; Gavin E Reid[1]; *[1]University 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. Couch[1]; Jayleigh M. Lanza[2]; Christopher M. Zall[2]; J. Tyler Davidson[1]; *[1]Department of Forensic Science, Sam Houston State University, Huntsville, TX; [2]Department 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 Davoli[1]; Alice Passoni[1]; Claudio Medana[2]; Enrica Mecarelli[2]; Victor Laiko[3]; Vladimir Doroshenko[3]; *[1]Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy; [2]Universita' degli Studi di Torino, Torino, Italy; [3]MassTech 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]; Grégoire Delaporte[3]; Christine Albaret[3]; Emmanuel Joubert[3]; Anne Bossée[4]; Laurent Debrauwer[1, 2]; Emilien L Jamin[1, 2]; *[1]Toxalim (Research Center in Food Toxicology), Toulouse university, INRAE, ENVT, INP-Purpan, Toulouse, France; [2]MetaboHUB-MetaToul, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France; [3]Analytical Chemistry Department, DGA CBRN Defence, 5 rue Lavoisier, Vert-Le-Petit, France; [4]Chemistry 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 Sisco[1]; Arun Moorthy[1]; *[1]NIST, Gaithersburg, MD*

WP 217 **Liquid Chromatographic High Resolution Accurate Mass Characterization of Polydimethylsiloxanes on Condoms and Sexual Lubricants**; B. Mckay Allred[1]; James Adams[1]; Joshua Little[2]; *[1]USACIL, Forest Park, GA; [2]ORISE - 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 Mironenka[1]; Anna Lenartowicz[1]; Adrian Soboń[1, 2]; Rafał Szewczyk[1, 2]; Katarzyna Krupczyńska-Stopa[1, 2]; Maciej Stopa[1, 2]; Andrzej Kwaśnica[3]; *[1]LabExperts sp. z o. o., Gdańsk, Poland; [2]Bioanalytic sp. z o. o., Gdańsk, Poland; [3]Lab4Tox sp. z o. o., Wrocław, Poland*

WP 219 **Molecular investigation of benzodiazepines in human blood by DART ionization and High-Resolution Mass Spectrometry**; Cecília A. Bhering[1]; Ananda S. Antonio[1]; Gleicielle T. Wurzler[1]; Alexandre N. P. Aguiar[1]; Diego R. Carvalhosa[2]; Antônio C. G. Jardim[3]; Marc Y. Chalom[3, 4]; Francois Espourteille[5]; Julio C. G. Silva[6]; Francisco R. A. Neto[1]; Gabriela V. Costa[1]; *[1]Universidade Federal do Rio de Janeiro, Instituto de Química, NAF – LADETEC, Rio de Janeiro, Brazil; [2]PCERJ, SEPOL, Instituto Médico Legal Afrânio Peixoto (IMLAP), Rio de Janeiro, Brazil; [3]SENS Advanced Mass Spectrometry, São Paulo, Brazil; [4]Consultancy, SÃO PAULO, Brazil; [5]Bruker Scientific, Billerica, MA; [6]Nova Analítica, São Paulo, Brazil*

WP 220 **Application of DART ionization in the forensic investigation of pesticide poisoning**; Gleicielle T. Wurzler[1]; Ananda S. Antonio[1]; Cecília A. Bhering[1]; Thamara A. Barra[1]; Alexandre N. P. Aguiar[1]; Diego R. Carvalhosa[2]; Antônio C. G. Jardim[3]; Marc Y. Chalom[3, 4]; Julio C. G. Silva[5]; Francois Espourteille[6]; Francisco R. A. Neto[1]; Gabriela V. Costa[1]; *[1]Universidade Federal do Rio de Janeiro, Instituto de Química, NAF – LADETEC, Rio de Janeiro, Brazil; [2]PCERJ, SEPOL, Instituto Médico Legal Afrânio Peixoto (IMLAP), Rio de Janeiro, Brazil; [3]SENS Advanced Mass Spectrometry, São Paulo, Brazil; [4]Consultancy, SÃO PAULO, Brazil; [5]Nova Analítica, São Paulo, Brazil; [6]Bruker Scientific, Billerica, MA*

WP 221 **Application of Machine-learning to Predict Physical Activity from Endogenous Fingerprint Compounds**; Daphne R Patten[1]; Trevor T Forsman[1]; Andrew E Paulson[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

WP 222 **Using High Resolution Mass Spectrometry to clarify ambiguous Benzodiazepine ions in the NIST EI-MS Library**; Edward Erisman[1]; Arun Moorthy[1]; William E. Wallace[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

WP 223 **Comparing Peptide Sequence Accuracy of MRM to Peptide Spectra Searching**; Heyi Yang[1]; Erin Butler[1]; Iyman Almubarak[1]; Tatiana Perez[1]; Jahaira Zapata[1]; Donald Siegel[1]; *[1]Office 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 Lattouf[1]; Aleksei Shcherbinin[2]; Juha Kangasluoma[2, 3]; Paxton Juuti[2]; Jussi Kontro[2]; Joona Mikkilä[2]; Jyri Mikkilä[2]; H.j. Jost[2]; *[1]Research scientist/Scientific Sales Lead, Helsinki, Finland; [2]Karsa Ltd., Helsinki, Finland; [3]Institute 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*

WP 226 **Van de Graaff generators as combined sampling devices and ion sources for non-contact mass spectrometry analysis of evidentiary materials**; Kenyon Evans-Nguyen[1]; Madison Autrey[1]; *[1]University of Tampa, Tampa, FL*

WP 227 **Rapid Characterization of Alkaloids using Probe ESI Q-TOF LCMS-9050 in OAD-MS/MS**; Hidenori Takahashi[1]; Kaoru Nakagawa[1]; Mami Okamoto[1]; Yuta Miyazaki[1]; Yohei Arao[1]; Tetsuo Iida[1]; *[1]SHIMADZU Corporation, Kyoto, Japan*

WP 228 **High-speed analysis of drugs of abuse in urine using Acoustic Ejection Mass Spectrometry**; Anuja Bhalkikar[1]; Jacob Watson McCabe[1]; Han Joo Lee[1]; Rahul Baghla[2]; Casey W. Burrows[1]; Alexandre Wang[1]; *[1]SCIEX, Frammingham, MA; [2]SCIEX, 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 Letarte[1]; Hugues Sinnett[1]; Serge Auger[1]; Jean Lacourcière[1]; Jonathan Rochon[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC*

WP 230 **Extraction of Illicit Drugs from Wastewater using a Solid Phase Extraction Syringe-cartridge Capsule**; Michael Apsokardu[1]; Xiaohui Zhang[1]; Guotao Lu[1]; *[1]CDS 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. Sanders[1]; Kimber N. Focke[2]; Michael T Marty[2]; *[1]University of Arizona, Tucson, AZ; [2]University of Arizona, Tuscon, 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]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Resource 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 Vink[1]; Jonathan Martens[1]; Wybren Jan Buma[2]; Giel Berden[1]; Jos Oomens[1]; *[1]FELIX Radboud University, Nijmegen, Netherlands; [2]University 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. Houthuijs[1]; Jonathan K. Martens[1]; Giel Berden[1]; Vasuk Gautam[2]; David S. Wishart[2]; Jos Oomens[1]; *[1]Radboud University Nijmegen, Nijmegen, Netherlands; [2]University of Alberta, Edmonton, AB*

WP 237 **Design of an Optical Ion Trap (OIT) Mass Analyzer**; Liam Dugan[1]; Frederick Lanni[1]; Mark E Bier[1]; *[1]Carnegie 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 Schultz[1]; Neil A. Ellis[1]; Maleesha T. Fernando[1]; Miyuru M. Wellalage[1]; Daniel A. Thomas[1]; *[1]University 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 Abeysooriya[1, 2]; Kie T. Workman[1, 3]; Wilson Gichuhi[1]; *[1]Department of Chemistry, Tennessee Tech University, 1 William L. Jones Dr., Cookeville, TN 38505; [2]School of Environmental Studies,Tennessee Tech University, Cookeville, TN 38505; [3]Department 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 Dossmann[3]; Denis Duflot[4]; *[1]Synchrotron Soleil, Gif-Sur-Yvette, France; [2]INRAE, UAR1008, Transform Department, Rue de la Géraudière, BP 71627,44316 Nantes, France, Nantes, France; [3]Sorbonne Université, Faculté des Sciences et de l'Ingénierie, Institut Parisien de Chimie Moléculaire (IPCM), Paris, France; [4]Université 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 Wan[1]; Haocheng Qian[1]; František Tureček[1]; *[1]University 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 Fernando[1]; Miyuru M Wellalage[1]; Emily M Molino[1]; Madeline Schultz[1]; Neil Ellis[1]; Daniel A Thomas[1]; *[1]University 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 Wellalage[1]; Maleesha T Fernando[1]; Emily M Molino[1]; Madeline Schultz[1]; Neil Ellis[1]; Daniel A Thomas[2]; *[1]University of Rhode Island, Kingston, RI; [2]University 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 Favre[1]; Igor Kaltashov[1]; *[1]UMASS Amherst, Amherst, MA*

WP 245 **Exploring Emitters for Generating ultra-low Current Electrospray Ionization**; Ian T Ferraro[1]; Huishan Li[1]; Nicholas Allen[1]; Taoqing Wang[1]; Anyin Li[1]; *[1]Department of Chemistry, University of New Hampshire, Durham, NH*

WP 246 **Ionization Efficiency of Glycans, Proteins and Subunits in femto Electrospray Modes**; Huishan Li[1]; Nicholas Allen[1]; Taoqing Wang[1]; Ian T Ferraro[1]; Mengtian Li[1]; Anyin Li[1]; *[1]University of New Hampshire, Durham, NH*

WP 247 **Elevation of the baseline in Quadrupole Mass Spectrometers: Mechanism and Solution**; Markus Langner[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

WP 248 **Mapping Nano-Electrospray Ionization Plumes on an Orbitrap Fusion Lumos Tribrid Mass Spectrometer Equipped with FAIMS**; Joshua A Silveira[1]; Gary A Schultz[1]; Kristina Rucker[1]; Yuan Lin[1]; Matt Tsai[1]; Michael Belford[1]; Cornelia Boeser[1]; Eloy R Wouters[1]; *[1]Thermo 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 Grooms[1]; Abraham K. Badu-Tawiah[1]; *[1]The 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 Heintz[1]; Oliver Braubach[1]; Walter Wissdorf[1]; Lisa Schnödewind[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

WP 251 **Observation of charged ESI droplets aspirated into the vacuum system of a commercial QIT under variated LC conditions**; Patricia Itzenhäuser[1]; Laura Lehmann[1]; Walter Wissdorf[1]; Ferdinand Wachter[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University 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 Devor[1]; Jing Wang[1]; Madison Pursell[1]; Olanrewaju Awoyemi[1]; Stephen Valentine[1]; Peng Li[1]; *[1]West Virginia University- C. Eugene Bennett Department of Chemistry, Morgantown, WV*

WP 253 **Gas-phase oxidation of benzaldehyde to benzoic acid under electrospray ionization mass spectrometric conditions**; Shimin He[1]; Sihang Xu[1]; Athula Attygalle[1]; *[1]Stevens Institute of Technology, Hoboken, New Jersey*

WP 254 **Thermal-Desorption Electrospray-Mass Spectrometry (TD-ESI-MS) for Dye Analysis**; Jiarui Rachel Wu[1]; Xinyi Sui[1]; Brian Musselman[2]; Nelson R Vinueza[1]; *[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 Stappert[1, 2]; 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 Bulut[1]; Chris Vico Heintz[1]; Walter Wissdorf[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

WP 257 **Feeding the ALPACA: Testing the Performance of Charge-Induction Amperometry of Electrosprayed Particles**; Cristian A. Blanco-Combariza[1]; Jeffrey E Dick[2]; *[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 Neumark[1]; Oneg Elkabets[1]; 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 Yakovchuk[1]; Alexander Gordin[1]; Aviv Amirav[1]; *[1]Tel Aviv University, Tel Aviv, Israel*

WP 260 **Open Probe Ultra-Fast GC-MS on the Bench for Improved Real Time Analysis**; Oneg Elkabets[1]; Benny Neumark[1]; 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 Ji[1]; Zhenyu Jin[1]; *[1]University of Kentucky, Lexington, KY*

WP 262 **Differential analysis of soil using GC Orbitrap MS and Compound Discoverer**; Dominic Roberts[1]; Xin Zheng[2]; Lukasz Rajski[3]; Nicholas Warner[3]; Daniel Kutscher[3]; Jason Cole[2]; *[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 Sanig[1]; Bryan C. Katzenmeyer[2]; Cristian Cojocariu[1]; Jeff Goshawk[1]; Agnieszka Kalinowska[3]; Christoph Rethmann[3]; Pascal Tuszewski[3]; Lindsay Hatch[2]; *[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 Huang[1]; Snow Bai[1]; Larry Shayne Greem[1]; Peilin Yang[1]; *[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 Kubo[1]; Azusa Kubota[1]; Masaaki Ubukata[1]; Timothy Bergeron[2]; *[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 Kubota[1]; Masaaki Ubukata[1]; Ayumi Kubo[1]; Kenji Nagatomo[1]; John Gonzales[2]; *[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 Satoh[1]; Masaaki Ubukata[1]; Azusa Kubota[1]; Ayumi Kubo[1]; Robert A. Dipasquale[2]; *[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 Roberts[1]; Jason Cole[2]; Lukasz Rajski[3]; Xin Zheng[2]; Pablo Miralles[4]; Clara Coscolla[4]; *[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 Qiu[1]; Anna Lundquist[2]; Aida Zuberovic Muratovic[3]; Kumari Ubhayasekera[1]; Jonas Bergquist[1]; *[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. Thomas[1]; Colton Myers[2]; Jason Herrington[2]; Kevin A. Schug[1]; *[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 Ji[1]; Lewis Y. Geer[1]; Nirina Rabe Andriamaharavo[1]; Yufang Zheng[1]; Edward P. Erisman[1]; H. Martin Garraffo[1]; James Little[1]; Gary Mallard[1]; Sanford P. Markey[1]; Yuri A. Mirokhin[1]; Quan-Long Pu[1]; Dmitrii V. Tchekhovskoi[1]; Nino G. Todua[1]; Oleg V. Toropov[1]; Kirill V. Tretyakov[1]; William E. Wallace[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

WP 272 **Using Hydrogen as Carrier Gas for GC/MS Analysis: GCxGC-HR-TOFMS with Multi-Mode Ion Source**; George Tikhonov[1]; Scott Pugh[1]; Vyacheslav Artaev[1]; *[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 Pu[1]; Yufang Zheng[1]; Kirill V. Tretyakov[1]; Edward P. Erisman[1]; *[1]NIST, Gaithersburg, MD*

WP 274 **Measurement and Evaluation of Plant Derived Compounds for a Comprehensive Electron Ionization MS Library**; Nirina Rabe Andriamaharavo[1]; Mak D. Tytus[2]; Weihua Ji[1]; William E. Wallace[2]; Stephen E. Stein[1]; *[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 Hao[1]; Dan Cardin[1]; John Quintana[1]; Tim Raub[1]; *[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 Raub[1]; Dan Cardin[1]; Weier Hao[1]; John Quintana[1]; *[1]Entech Instruments, Simi Valley, CA*

WP 277 **Helium to Hydrogen: Explosives & Pesticides & VOAs, Oh My! Successful Transition of GC/MS Analyses**; Eric Fausett[1]; Anastasia Andrianova[2]; Bruce Quimby[3]; Angela

Smith Henry[3]; Kirk Lokits[2]; Limian Zhao[2]; Jessica Westland[4]; Samuel P Haddad[4]; Aaron Boice[5]; *[1]Agilent, Landenberg, PA; [2]Agilent Technologies, Wilmington, DE; [3]Agilent Technologies, Wilmington, Delaware; [4]Agilent Technologies, Wilmington; [5]Agilent 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 Quintana[1]; Dan Cardin[1]; Weier Hao[1]; Tim Raub[1]; *[1]Entech 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 Saldana[1]; Jacqueline Brummett[1]; Patrick Jensen[1]; *[1]Yakima Chief Hops - Yakima, WA, Yakima, WA*

WP 280 **Bench Scale Py-GC/MS with In-Line Reactor for Predicting Arrhenius Parameters**; Jeffrey Michael McGuire[1]; John C Carpin[2]; *[1]U.S. Army DEVCOM Chemical Biological Center, Aberdeen Proving Ground, MD; [2]EXCET 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 Deyanova[1]; David Weis[1]; *[1]Bristol-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 Lento[2]; Ayesha Maqsood[2]; Derek Wilson[2]; *[1]Emeritus, Brampton, ON; [2]York 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 Langford[1]; Mulin Fang[1]; Kellye A. Cupp-Sutton[1]; Jake Kline[1]; Luca Fornelli[1]; Si Wu[1]; *[1]University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK*

WP 284 **HILIC separations for HDX-MS at subzero temperatures**; Kyle W Anderson[1]; Jeffrey W Hudgens[1]; *[1]NIST, Rockville, MD*

WP 285 **deMix_GUI: A software package for automated HDX-MS data analysis and interrogation**; Hyeyoun Jung[1]; Seungjin Na[2]; Eunok Paek[2]; *[1]Grinnell College, Grinnell, IA; [2]Hanyang 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 Lambert[1]; Marius Gramlich[2]; Luke Smith[3]; Luisa Stutzke[1]; Dingyu Deng[1]; Philipp Kaiser[2]; Alesi Escobedo[4]; Ellie James[4]; Mike Guttmann[4]; Justin LP Benesch[3]; Ulrich Rothbauer[2]; Maximiliane Koenig[5]; Cornelia Wagner[5]; Pavla Vankova[6]; Petr Pompach[6]; Petr Novak[7]; Anne Zeck[2]; Kasper D. Rand[1]; *[1]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; [2]NMI Natural and Medical Sciences Institute at the University of Tübingen, Reutlingen, Germany; [3]Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, United Kingdom; [4]Department of Medicinal Chemistry, University of Washington, Seattle, Washington; [5]Roche Pharma Research and Early Development, Large Molecule Research, Penzberg, Germany; [6]BioCeV - Institute of Biotechnology of the CAS, Prague, Czech Republic; [7]BioCeV - 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. Hansen[1]; Rasmus R. Svejdal[1]; Jack Barrett[1]; Jörg P. Kutter[1]; Kasper D. Rand[1]; *[1]Department 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 Filandr[1]; Vladimir Sarpe[1]; Shaunak Raval[1]; Morgan Khan[1]; Pauline Douglas[1]; Yuqi Shi[2]; Rosa Viner[2]; Stephen Coales[3]; David Schriemer[1]; *[1]University of Calgary, Calgary, AB; [2]Thermo Fisher Scientific, San Jose, CA; [3]Trajan Scientific & Medical - Raleigh, Morrisville, NC*

WP 289 **A fully automated HX-DIA data analysis workflow for whole proteome deuteration experiments**; Vladimir Sarpe[1]; František Filandr[1]; D Alex Crowder[1]; David C Schriemer[1]; *[1]University of Calgary, Calgary, AB*

WP 290 **Histidine hydrogen-deuterium exchange (His-HDX) mass spectrometry for identifying protein-ligand interactions**; Kouhei Tanaka[1]; Tarou Kishimoto[1]; Shinko Watanabe[1]; Kaori Mitsui[1]; Chieko Okumura[1]; Kouta Murasaki[1]; Masaru Miyagi[2]; Ayako Kurimoto[3]; Sen Ilker[3]; *[1]Mitsubishi Tanabe Pharma Corporation, Kanagawa, Japan; [2]Case Western Reserve University, Cleveland, OH; [3]Protein Metrics, LLC, Cupertino, CA*

WP 291 **Nylon membrane immobilized acid protease digestion for hydrogen deuterium exchange capillary electrophoresis mass spectrometry**; Jordan Aerts[1]; Per E. Andren[1]; Erik T Jansson[1]; *[1]Uppsala University, Uppsala, Sweden*

WP 292 **Millisecond hydrogen/deuterium-exchange mass spectrometry of tryptophan side chains**; Jess Ramsay[1]; Dr Daniel Kattnig[1]; Dr Jonathan Phillips[1]; *[1]University 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-Sutton[1]; Thomas Welborn[1]; Mulin Fang[1]; Joel Langford[1]; Si Wu[1]; *[1]University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK*

WP 294 **Cross-Platform Standardization of Gas-Phase Hydrogen/Deuterium Exchange**; Alesi R Escobedo[1]; Sunjit S. Uppal[1]; Mike Guttmann[1]; *[1]University of Washington, Seattle, WA*

WP 295 **New tools for aid with the analysis of bimodal HDX-MS data**; Miklos Guttman; *University 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. Ferrari[1]; Sugyan M Dixit[1]; Jane M Thibeault[1]; Gabriel J Rocklin[1]; *[1]Northwestern University, Chicago, IL*

WP 297 **HDX-MS with in-line electrochemical reduction of disulfide bonds – state of the art**; Hendrik-jan Brouwer[1]; Jean-Pierre Chervet[1]; Martin Eysberg[2]; *[1]Antec Scientific, Alphen a/d Rijn, Netherlands; [2]Antec Scientific, Bostson, MA 02108*

WP 298 **Operation at Constant Ultrahigh Resolution with 2ωDetection using the Dynamically Harmonised Cell**; Benedict Gannon[1]; Diana C Palacio Lozano[1]; Hugh E Jones[1]; Mark P. Barrow[1]; *[1]University of Warwick, Coventry, United Kingdom*

WP 299 **Handling the noticeable non-linearity of mass calibration in High resolution ToF MS**; Boris Kozlov[1]; Sergey Kirillov[2]; *[1]Waters, Wilmslow, United Kingdom; [2]MSC-CG Ltd, Bar, Montenegro*

WP 300 **Increased sensitivity and throughput for native intact mass analysis using an online buffer exchange column**; Reiko Kiyonami[1]; Weijing Liu[1]; Rosa Viner[1]; Min Du[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo 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 Hsu[1]; Chao-Yi Chen[1, 2]; Tzu-Yu Pan[1]; Acharee Kaewlaoyoong[1]; Min-Zong Huang[1]; Chia-Fang Wu[1, 2]; *[1]Research Center for Precision Environmental Medicine, Kaohsiung Medical University, Kaohsiung city, Taiwan; [2]International Master Program of Translational Medicine, National United University, Miaoli city, Taiwan*

WP 302 **Comprehensive analysis of instrument parameters to achieve high-level ion focusing in linear time-of-flight mass spectrometry**; Yi-Hong Cai[1]; Yi-Sheng Wang[1]; *[1]Genomics 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 Xuan[1]; Anna Pashkova[1]; Martin Zeller[1]; Colin Tobias Wirth[1]; Jens Grote[1]; Andreas Kuehn[1]; Tabiwang N. Arrey[1]; Eugen Damoc[1]; Sally Webb[2]; Thomas Moehring[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo 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 Hain[1]; Kathleen Luo[1]; Om Shrestha[1]; Christopher Gilles[1]; Evelyn Wang[1]; Xiaomeng Xia[1]; Robert English[1]; Tiffany Liden[1]; *[1]Shimadzu 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 Tiemann[1]; Lukas Schwalb[1, 2]; Christopher Paul Rüger[1]; Martha Liliana Chacón-patiño[3]; Thomas Gröger[2]; Ralf Zimmermann[1, 2]; *[1]Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; [2]Joint Mass Spectrometry Centre (JMSC), Cooperation Group "Comprehensive Molecular Analytics" (CMA), Helmholtz Zentrum München GmbH, German Research Center for Environmental Health, Neuherberg, Germany; [3]National High Magnetic Field Laboratory, Tallahassee, FL*

WP 306 **Qualitative and quantitative analysis of Organic Solvents in lithium battery electrolysis by LC-QTOF**; Haiyang Wang[1]; Zhihui Lin[1]; Jianzhong Li[2]; Peibin Hu[3]; *[1]Agilent Technologies, Inc, Guangdong, China; [2]Agilent Technologies, Inc, Beijing, China; [3]Agilent Technologies, Inc, Chengdu, China*

WP 307 **Determination of Oxytocin in the mouse brain by HR-UHPLC-MS: Method Development and Validation**; Hanin Diab[1]; Jonathan Thompson[2]; Klementina Fon Tacer[2]; Tara Bayat[2]; *[1]Texas Tech University, Amarillo, TX; [2]School 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 Hock[1]; Hamish Stewart[1]; Eduard Denisov[1]; Amelia Peterson[1]; Nicolaie Eugen Damoc[1]; Martin Zeller[1]; Tabiwang N. Arrey[1]; Anna Pashkova[1]; Alexander Wagner[1]; Wilko Balschun[1]; Alexander Kholomeev[1]; Dmitry Grinfeld[1]; Alexander A Makarov[1]; *[1]Thermo 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. Sohn[1]; David C Muddiman[1]; *[1]North 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 Lin[1]; Haiyang Wang[1]; Jianzhong Li[2]; Peibin Hu[3]; *[1]Agilent Technologies, Inc, Guangzhou, China; [2]Agilent Technologies, Inc, Beijing, China; [3]Agilent 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 Lee[1]; Se Hee Hong[1]; Sang Beom Han[1]; *[1]Department 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 McCullagh[1]; Stephen Griffin[2]; Emma Marsden-Edwards[1]; David Eatough[1]; Dale Cooper-Shepherd[1]; Martin Palmer[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters 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 McCullagh[1]; Iggy Kass[2]; Emma Marsden-Edwards[1]; David Eatough[1]; Dale Cooper-Shepherd[1]; Martin Palmer[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters, 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 Friederici[1]; Anika Neumann[1]; Arne Koch[1]; Martha Liliana Chacón-patiño[2, 3]; Paolo Bomben[4]; Thorsten Streibel[1, 5]; Murray Gray[4, 6]; Ralf Zimmermann[1, 5]; *[1]Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; [2]International Joint Laboratory - iC2MC: Complex Matrices Molecular Characterization, TRTG, Harfleur, France; [3]National High Magnetic Field Laboratory, Tallahassee, FL; [4]Alberta Innovates, Calgary, AB; [5]Joint Mass Spectrometry Center, Cooperation Group Comprehensive Molecular Analytics, Helmholtz Zentrum München, German Research Center for Environmental Health, Neuherberg, Germany; [6]University of Alberta, Edmonton, AB*

WP 315 **Unveiling the performance of a novel high-resolution accurate mass platform for proteomics applications**; Tabiwang N. Arrey[1]; Amirmansoor Hakimi[2]; Eduard Denisov[1]; Nicolaie Eugen Damoc[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo 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 Park[1]; Stephen Dearth[2]; Hai Pham-Tuan[2]; Agnes Scharrer[2]; Vyncent Nguyen[3]; Didar Asik[3]; Chengjian Tu[3]; Ronny Dosanjh[1]; John Point[1]; George Bu[1]; Elizabeth C Dodson[1]; *[1]Thermo Fisher Scientific, Hunt Valley, MD; [2]Biocrates Life Sciences AG, Innsbruck, Austria; [3]Thermo Fisher Scientific, Grand Island, NY*

WP 317 **Evaluation of a novel Tribrid Orbitrap Ascend system for in-depth high-throughput proteomics and phosphoproteomics**; Yuchen He[1]; Katherine Overmyer[1, 2]; Dain R. Brademan[1, 2]; David Bergen[3]; Jingjing Huang[3]; Romain Huguet[3]; Michael W. Senko[3]; Vlad Zabrouskov[3]; Michael S. Westphall[1]; Evgenia Shishkova[1]; Graeme C McAlister[3]; Joshua J. Coon[1, 2]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Morgridge Institute for Research, Madison, WI; [3]ThermoFisher 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 Hanna[1]; Ziqin Ni[2]; Adrian Southard[2]; Ricardo Arevalo Jr. [3]; *[1]University of Maryland, College Park, MD; [2]University of Maryland College Park, College Park, MD; [3]University 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 Zemaitis[1]; Eric Choi[1]; Rosalie Chu[1]; Yuri E. Corilo[1]; Sai Munikoti[2]; Jordan Rabus[1]; Jan Strube[2]; William Kew[1]; *[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington 99354; [2]Pacific Northwest National Laboratory, Richland, WA*

WP 320 **Urinary Forensic Toxicology Data Independent Analysis Screening: Using High Resolving Power Multi-Reflecting Time-of-Flight Mass Spectrometry**; Michael McCullagh[1]; Johannes PC Vissers[1]; Martin Palmer[1]; Jane Cooper[1]; Michelle Wood[1]; Emma Marsden-Edwards[1]; Nayan Mistry[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

WP 321 **New Tribrid MS ion optics and electronics improve sensitivity, duty cycle, and extend the MS range**; Graeme McAlister[1]; Xiao Wang[1]; Mike Goodwin[1]; Christopher Mullen[1]; Jesse D. Canterbury[1]; Raman Mathur[1]; Romain Huguet[1]; David Bergen[1]; Jingjing Huang[1]; Michael W. Senko[1]; Vlad Zabrouskov[1]; *[1]Thermo 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 Lin[1]; Manal L. Zabalawi[2]; Lane M. Smith[3]; Peter W. Stacpoole[4]; Charles E. McCall[2]; Boone M. Prentice[1]; *[1]Department of Chemistry, University of Florida, Gainesville, FL; [2]Department of Internal Medicine/Molecular Medicine and Department of Microbiology and Immunology, Wake Forest School of Medicine, Winston-Salem, NC; [3]Department of Anesthesiology, University of Michigan Medical School, Ann Arbor, MI; [4]Department 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. Claes[1]; Annet A.M. Duivenvoorden[1]; Caitlin M. Tressler[2]; Ethan Yang[2]; Kanchan Sonkar[2]; Shane R. Ellis[1, 3]; Kristine Glunde[2]; Ron M.a. Heeren[1]; *[1]Maastricht University, Maastricht, Netherlands; [2]Johns Hopkins University School of Medicine, Baltimore, MD; [3]University 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 Passoni[1]; Angela Marika Siciliano[1]; Monica Favagrossa[1]; Alessia Lanno[1]; Laura Colombo[1]; Mario Salmona[1]; Renzo Bagnati[1]; Enrico Davoli[1]; *[1]Istituto 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 Paez[1]; Sadhana Chauhan[1]; Kubra F. Naqvi[2]; Janice Endsley[1]; Brendan Prideaux[1]; *[1]University of Texas Medical Branch, Galveston, TX; [2]University 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 Guo[1]; Shuli Tang[1]; Jiaxin Feng[1]; Luchen Wuyang[1]; Xin Yan[1]; *[1]Texas 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 Zhang[1]; Leila Hejazi[1, 2]; Petter Bjornstad[3]; Hak Joo Lee[1]; Nerlyn Garcia Ponce De Leon[1]; Christopher R. Anderton[4]; Theodore Alexandrov[5]; Manjeri A. Venkatachalam[1]; Kumar Sharma[1]; *[1]UT Health San Antonio, San Antonio, TX; [2]SygnaMap, Inc., San Antonio, TX; [3]University of Colorado Anschutz Medical Campus, Aurora, CO; [4]Pacific Northwest National Laboratory, Richland, WA; [5]European 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 Okuda[1]; Ei-ichi Matsuo[1]; Jeffrey Dahl[2]; Toshiya Matsubara[2]; Shinichi Yamaguchi[1]; Jannine I. Gamayot[3]; Shiuhwei Chen[3]; Christine M. Kusminski[3]; Philipp E. Scherer[3]; Ruth Gordillo[3]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Scientific Instrument, Columbia, Maryland; [3]University 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 Wiedemann[1]; Stefanie Gerbig[1]; Parviz Ghezellou[1]; Nils H Anschütz[1]; Alejandra Peter Ventura[1]; Martin Roderfeld[2]; Elke Roeb[2]; Thomas Quack[3]; Christoph G Grevelding[3]; Liliana M R Silva[3]; Carlos R Hermosilla[3]; Anja Taubert[3]; Kerstin Strupat[4]; Bernhard Spengler[1]; *[1]Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, 35392 Giessen, Germany; [2]Gastroenterology, Justus Liebig University Giessen, 35392 Giessen, Germany; [3]Institute of Parasitology, Justus Liebig University Giessen, 35392 Giessen, Germany; [4]Thermo 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]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Nephrology, Department of Medicine, Vanderbilt University Medical Center, Nashville, TN; [5]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, Nashville, TN; [6]Department of Pediatrics, Vanderbilt University Medical Center, Nashville, TN; [7]Department of Chemistry, Vanderbilt University, Nashville, TN*

WP 332 **MALDI HiPLEX-IHC on Tissue Microarrays in Neuropathology Research**; Yasemin Ucal[1]; D.r. Naomi Vos[1]; S. Alexandra Iakab[1]; Henri Bogumil[2]; Rouzbeh Benan[2]; Gargey B. Yagnik[3]; Signe Frost Friedricksen[4]; Corinna Henkel[4]; Mark Lim[3]; Andreas Von Deimling[2, 5]; Carsten Hopf[1, 6]; *[1]Center for Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim University of Applied Sciences, Mannheim, Germany; [2]Department of Neuropathology, Institute of Pathology, Heidelberg University Hospital, Heidelberg, Germany; [3]AmberGen, Inc., Billerica, MA; [4]Bruker Daltonik GmbH, Bremen, Germany; [5]Klinische Kooperationseinheit Neuropathologie, Deutsches Krebsforschungszentrum (DKFZ), Heidelberg, Germany; [6]Medical Faculty, Heidelberg University, Heidelberg, Germany*

WP 333 **Imaging Mass Spectrometry Analysis of Gastric Proteome Changes after Helicobacter Pylori Infection in Gerbils**; Michelle L. Reyzer[1]; Jennifer Shuman[1]; Audra M. Judd[1]; Hayes McDonald[1]; Kevin L. Schey[1]; Timothy L. Cover[1, 2]; Richard M Caprioli[1]; *[1]Vanderbilt University, Nashville, TN; [2]Veterans Affairs Tennessee Valley Health Care System, Nashville, TN*

WP 334 **Multimodal Mass Spectrometry Imaging of Key Biomarkers To Study Ocular Disease**; Joshua J O Millar[1]; Susan Campbell[1]; Catherine Duckett[1]; Sarah Doyle[2]; Laura Cole[1]; *[1]Sheffield Hallam University, Sheffield, United Kingdom; [2]Trinity College Dublin, Dublin, Ireland*

WP 335 **Imaging of Fatty Acids in Brains Influenced by Cannabis and the Control of Unwanted Lipid Fragmentation**; Samantha L. Cousineau[1]; Mohammed H. Sarikahya[1]; Kristina Jurcic[1]; Steven R. Laviolette[1]; Ken K.-C. Yeung[1]; *[1]University 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 Chen[1]; Jarod Fincher[1]; Mark Cancilla[1]; *[1]Merck, West Point, PA*

WP 337 **Enhancement of Lipid Signals in Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry with**

Ammonium Fluoride as a Matrix Additive; Joseph H. Holbrook[1]; Emily R. Sekera[2]; Arbil Lopez[2]; Brian D. Fries[2]; Fernando Tobias[2]; Kubra Akkaya[3]; Maria M. Mihaylova[1, 3, 4]; Amanda B. Hummon[1, 2, 4]; *[1]The Ohio State University-Ohio State Biochemistry Program, Columbus, OH; [2]The Ohio State University-Department of Chemistry and Biochemistry, Columbus, OH; [3]The Ohio State University-Department of Biological Chemistry and Pharmacology, Columbus, OH; [4]The Ohio State University-Comprehensive Cancer Center, Columbus, OH*

WP 338 **Label-Free High-Resolution Molecular Imaging of Stratum Corneum by Cluster Secondary Ion Mass Spectrometry (Cluster SIMS)**; Naoko Sano[1]; Kate McHardy[1]; Paul Blenkinsopp[1]; *[1]Ionoptika 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 Claude[1]; Nyasha Munjoma[1]; Alex Birsan[2]; Ian D Wilson[3]; Joanne B Ballantyne[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Limited, Quebec, N/A; [3]Division 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 Tabang[1]; Hua Zhang[2]; Daniel M. Tremmel[3, 4]; Sara Dutton Sackett[3]; Jon Odorico[3]; Lingjun Li[1, 2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Department of Surgery, University of Wisconsin-Madison, Madison, WI; [4]Department 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 Claude[1]; Farid Jahouh[2]; Martin E. Palmer[1]; Inneke Wynant[2]; Filip Cuyckens[2]; Marjolein Van Heerden[2]; Jan Claereboudt[3]; Rob J Vreeken[2, 4]; Lance Nicolaysen[5]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Preclinical Sciences & Translational Safety, Janssen R&D, Beerse, Belgium; [3]Waters Corporation, Antwerpen, Belgium; [4]Maastricht MultiModal Molecular Imaging Institute, Maastricht University, Maastricht, Netherlands; [5]Waters Corporation, Milford, MA*

WP 342 **Targeted Quantitative Analysis of the Effect of Fomepizole on Acetaminophen Nephrotoxicity with a DESI Tandem Quadrupole MS Imaging Platform**; Jephte Akakpo[1]; Anthony Midey[2]; Bindesh Shrestha[2]; Hartmut Jaeschke[1]; Anup Ramachandran[1]; *[1]University of Kansas Medical Center, Kansas City, KS; [2]Waters Corporation, Milford, MA*

WP 343 **Mapping Physiologically Relevant Concentrations of Morphine in the Brain by IR-MALDESI MSI**; Yury Desyaterik[1]; Austin M. Jones[2]; Kara M. Rademeyer[2]; Mary Peace McRae[2]; Angela D. M. Kashuba[1]; Elias P. Rosen[1]; *[1]UNC, Chapel Hill, NC; [2]Virginia Commonwealth University, Richmond, VA*

WP 344 **MALDI MSI visualizes the efficacy of cell therapy for treatment of mucopolysaccharidosis in murine brain**; Axel Treu[1]; Panagiotis Douvaras[2]; Tim Brandenburger[1]; Beate Schnippert[1]; Diego F. Buenaventura[2]; Ashley Lepack[2]; Christoph Patsch[2]; Uwe Thuss[1]; *[1]Bayer AG, Wuppertal, Germany; [2]BlueRock 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 Samal[1]; Tana V. Palomino[2]; Judy Chen[1]; David C Muddiman[2]; Tatiana Segura[1]; *[1]Duke University, Durham, NC; [2]North 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 Luh[1]; Sven Heiles[1, 2, 3]; Martin Roderfeld[4]; Christoph G. Grevelding[5]; Elke Roeb[4]; Kerstin Strupat[6]; Bernhard Spengler[1]; *[1]Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, 35392 Giessen, Germany; [2]Leibniz Institute for Analytical Sciences - ISAS - e.V., 44139 Dortmund, Germany; [3]Lipidomics, Faculty of Chemistry, University of Duisburg-Essen, 45141 Essen, Germany; [4]Gastroenterology, Justus Liebig University Giessen, 35392 Giessen, Germany; [5]Institute for Parasitology, Justus Liebig University Giessen, 35392 Giessen, Germany; [6]Thermo 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 Muller[1]; Nivedita Hegdekar[2]; Chinmoy Sarkar[3]; Marta M. Lipinski[3]; Maureen A. Kane[1]; *[1]University of Maryland, School of Pharmacy, Baltimore, MD; [2]University of Maryland, School of Medicine, Baltimore, MD; [3]University 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 Migas[3]; 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]; *[1]Department of Cell and Developmental Biology, 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]Vanderbilt University, Department of Biochemistry, Nashville, TN; [5]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [6]Department 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 Fernandez[5]; 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 Schrag[5, 8]; Jeffrey M Spraggins[1, 2, 3, 4, 6, 7]; *[1]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [3]Biomolecular Multimodal Imaging Center, Vanderbilt University, Nashville, TN; [4]Chemical Physical Biology Program, Vanderbilt University School of Medicine, Nashville, TN; [5]Department of Neurology, Vanderbilt University, Nashville, TN; [6]Department of Biochemistry, Vanderbilt University, Nashville, TN; [7]Department of Chemistry, Vanderbilt University, Nashville, TN; [8]Cerebral 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-Dávila[1]; Benjamin L. Oyler[1]; Richard Koup[1]; Constantinos Petrovas[1]; *[1]Tissue 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 Iqfath[1]; Manxi Yang[2]; Palak Manchanda[2]; Julia Laskin[2]; Gaurav Chopra[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, WEST LAFAYETTE, IN*

WP 352 **Exploring in vivo deuterium labeling in surface tissues of Arabidopsis thaliana using MALDI-MS imaging**; Sumin Na[1]; Young-Jin Lee[1]; *[1]Iowa State University, ames*

WP 353 **Examining the Metabolic Factors Promoting Clostridioides difficile infection in Inflammatory Bowel Disease through Imaging Mass Spectrometry.**; Troy R. Scoggins Iv[1]; Amanda Pebenito[2, 3]; Jonathan T. Specker[1];

Joseph P. Zackular[4, 5]; Boone M. Prentice[1]; *[1]Department of Chemistry, University of Florida, Gainesville, FL; [2]Division of Gastroenterology, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [3]Division of Protective Immunity, Children's Hospital of Philadelphia, Philadelphia, PA; [4]Division of Protective Immunity, Children's Hospital of Philadelphia, Philadelphia, PA; [5]Department of Pathology and Laboratory Medicine, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA*

WP 354 **Rapid and high spatial mapping of drugs by atmospheric pressure matrix-assisted laser desorption ionization mass spectrometry imaging**; Ariful Islam[1]; Md. Al Mamun[1]; Muedur Rahman[1]; Takumi Sakamoto[1]; Tomohito Sato[1]; Tomoaki Kahyo[1]; Yutaka Takahashi[1]; Mitsutoshi Setou[1]; *[1]Department 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 Pusparajah[1]; Margi Patel[1]; Berk U. Rasheed[1]; Krishna K. Singh[1]; Ken K.-C. Yeung[1]; *[1]Western University, London, ON*

WP 356 **Trace Level Quantification of Nitrosamine Impurities in Tuberculosis Medicines by LC-MS/MS**; Qiyao Li[1]; Qun Xu[1]; Nadine Lo[1]; Allan Leeks[1]; Mark Han[1]; Marcela Nefliu[1]; Jack Simpson[1]; Jennifer Belsky[1]; *[1]USP, Rockville, MD*

WP 357 **Native Datalake; enabling a Data Pipeline for Data Analysis with small to medium Native datasets**; Ryan P Marchand[1]; Richard Chapman[2]; Neil Landers[1]; *[1]Waters corp, milford, MA; [2]Waters 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 Du[1]; Tracy Zhou[1]; Sven Hackbusch[2]; Kelly Broster[3]; *[1]Genentech Inc., South San Francisco, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Hemel, United Kingdom*

WP 360 **Sequence confirmation and impurity characterization of therapeutic oligonucleotides – A quality by design approach**; Giovanni Calderisi[1]; Patrik Plattner[1]; Agron Selami[1]; *[1]Bachem AG, Bubendorf, Switzerland*

WP 361 **Enhanced screening for Active Pharmaceutical Ingredients (APIs) through the integration of a single quadrupole mass spectrometer**; Kathleen K Luo[1]; Ethan R Hain[1]; Om K Shrestha[1]; Evelyn H Wang[1]; Xiaomeng Xia[1]; Robert English[1]; Tiffany Liden[1]; Christopher Gilles[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

WP 362 **Quantitative Analysis of Azido Impurities in Five Sartan Drug Substances using a Triple Quadrupole Mass Spectrometer**; Kate (xiaomeng) Xia[1]; Logan Miller[1]; Evelyn H. Wang[1]; Tairo Ogura[1]; Yoshiyuki Okamura[1]; *[1]Shimadzu Scientific Instruments, Columbia, MD*

WP 363 **Novel Time-of-Flight Residual Gas Analyzer (TOF-RGA) for in situ Real-time Process Monitoring**; Lukas Hofer[1]; Sébastien Gasc[1]; *[1]Spacetek 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 Cappellin[1]; Luigi Ciotti[1]; Manuel Hutterli[1]; Michael Groessl[1]; *[1]TOFWERK, Thun, Switzerland*

WP 365 **An Improved Method for Quantifying Glyphosine Impurity in Glyphosate API using LC/MS/MS via Standard Addition**; Chun-Ye Sun[1]; Shao-Zhen Wang[1]; *[1]Agilent 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 Tarczynski[1]; Joanna Bis[1]; Elliott Franco[1]; Leslie Silva[2]; Vaughan Langford[3]; *[1]Alcami Corporation, Morrisville, NC; [2]Syft Technologies, Los Angeles, CA; [3]Syft Technologies, Christchurch Central City, New Zealand*

WP 368 **Operating, maintaining, and troubleshooting the sensitivity and robustness of timsTOF platforms for proteomics studies**; Benoit Fatou[1]; Conor Mullens[1]; Elizabeth Gordon[1]; Diego Assis[1]; Alvaro Sebastian Vaca[2]; Michael Krawitzky[2]; Matt Willetts[1]; *[1]Bruker Scientific LLC, Billerica, MA; [2]Bruker 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. Voyksner[1]; Paul Lorcheim[2]; *[1]LCMS Limited, Durham, NC; [2]ClorDiSys 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 Williams[1]; Leonard B Collins[1]; Sobhana Sripada[1]; Stefano Menegatti[1]; *[1]NCSU, Raleigh, NC*

WP 372 **PTM localization score MaxTopos for data-independent acquisition data in MaxQuant applied to phosphoproteomics provides accurate site localization**; Pelagia Kyriakidou[1]; Shamil Urazbakhtin[1]; Tanja Bange[2]; Maria Robles[2]; Juergen Cox[1]; *[1]Computational Systems Biochemistry Research Group, Max-Planck Institute of Biochemistry, Martinsried, Germany; [2]Institute of Medical Psychology and Biomedical Center, Faculty of Medicine, Ludwig-Maximilians-University, München, Germany*

WP 373 **XMass: XGBoost-based peptide spectral library prediction integrated into MaxQuant for DDA and DIA data analysis**; Shamil Urazbakhtin[1]; Favio Salinas-Soto[1]; Pelagia Kyriakidou[1]; Juan Luis Restrepo-Lopez[1]; Juergen Cox[1]; *[1]Computational 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 Murase[2]; Masaki Kato[2, 3]; Hiroyuki Yamamoto[2, 4]; Tsuyoshi Tabata[2, 5]; Maiko Kusano[2, 6]; Shin Kawano[2, 7]; Susumu Goto[8]; Yasushi Ishihama[5]; Akiyasu C. Yoshizawa[2, 5, 7]; *[1]Trans-IT Co., Ltd., Mibu-machi, Japan; [2]Mass++ Users Group, Kyoto, Japan; [3]Data Knowledge Organization Unit, RIKEN Information R&D and Strategy Headquarters, RIKEN, Wako, Japan; [4]Human Metabolome Technologies, Inc., Tsuruoka, Japan; [5]Grad. School of Pharma. Sci., Kyoto Univ., Kyoto, Japan; [6]School of Medicine, Showa Univ., Shinagawa, Japan; [7]Toyama Intl. Univ., Toyama, Japan; [8]DBCLS, DS, ROIS, Kashiwa, Japan*

WP 375 **Fully automated and spectrum-centric processing of parallel reaction monitoring (PRM) data**; Daniel P. Zolg[1]; Tobias Schmidt[1]; Siegfried Gessulat[1]; Florian Seefried[1]; Samia Ben Fredj[1]; Mathias Wilhelm[2]; Martin Heinrich Frejno[1]; *[1]MSAID GmbH, Garching b.München, Germany; [2]Computational 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 Zeinert[1]; Bernhard Y Renard[1]; Christoph N Schlaffner[1]; *[1]Data 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 Callens[1, 2]; Tine Claeys[1, 2]; Sander Willems[3]; Maarten Dhaenens[4]; Lennart Martens[1, 2]; *[1]VIB-UGent Center for Medical Biotechnology, Gent,* *Belgium; [2]Ghent University, Gent, Belgium; [3]Department of Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Martinsried, Germany; [4]Ghent University, Laboratory of Pharmaceutical Biotechnology, Ghent, Belgium*

WP 378 **midiaID: a spectra-centric pipeline for the analysis of the midiaPASEF data**; Mateusz Krzysztof Lacki[1]; Ute Distler[1]; Michał Piotr Startek[1, 2]; David Teschner[3]; Sven Brehmer[4]; Jens Decker[4]; Thilo Schild[5]; Jonathan R Krieger[6]; Florian Krohs[4]; Oliver Raether[4]; Andreas Hildebrandt[3]; Stefan Tenzer[5]; *[1]University Medical Center, Johannes Gutenberg University, Mainz, Germany; [2]Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Warsaw, Poland; [3]Institute for Informatics, Johannes-Gutenberg University, Mainz, Germany; [4]Bruker Daltonics GmbH & Co.KG, Bremen, Germany; [5]University Medical Center of Mainz, Mainz, Germany; [6]Bruker Ltd., Milton, ON*

WP 379 **dia-PASEF Tools: a shiny App for data visualization and exploration of dia-PASEF data**; Alvaro Sebastian Vaca[1]; Christopher Adams[1]; Matthew Willetts[2]; *[1]Bruker Scientific LLC, San Jose, CA; [2]Bruker Scientific, LLC, Billerica, MA*

WP 380 **Panorama Enhancements for System Suitability, Multi-Attribute Method, and Protein Coverage**; Josh Eckels[1]; Wendy Innis[1]; Ankur Juneja[1]; Sweta Jewargikar[1]; Nicholas Shulman[2]; Vagisha Sharma[2]; Michael J. MacCoss[2]; Brendan MacLean[2]; *[1]LabKey, San Diego, CA; [2]University of Washington, Seattle, WA*

WP 381 **A Protein Functional Map Learned from Pan-cancer Multi-Omics Data Enlightens Somatic Mutations, Understudied Genes, and Cancer Hallmarks**; Zhiao Shi[1]; Jonathan Lei[1]; Bing Zhang[1]; *[1]Baylor College of Medicine, Houston, TX*

WP 382 **Finding Cancer Hallmarks Through Changes in mRNA/protein Relationships**; Jose Humberto Giraldez Chavez[1]; Samuel H Payne[1]; *[1]Brigham Young University, Provo, UT*

WP 383 **Pan-cancer proteogenomics expands the landscape of therapeutic targets**; Jonathan T Lei[1]; Sara R Savage[1]; Xinpei Yi[1]; Bo Wen[1]; Hongwei Zhao[2]; Lauren K Somes[1]; Paul W Shafer[1]; Dou Yongchao[1]; Zhiao Shi[1]; Qiang Gao[2]; Valentina Hoyos[1]; Bing Zhang[1]; *[1]Baylor College of Medicine, Houston, TX; [2]Zhongshan 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 Abouelhassan[1]; Katherine A. Overmyer[2, 3]; Timothy W. Rhoads[4, 5]; Rozalyn M. Anderson[4, 5, 6]; Joshua J. Coon[2, 3, 7]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI; [3]Morgridge Institute for Research, Madison, WI; [4]Department of Nutritional Sciences, University of Wisconsin-Madison, Madison, WI; [5]Department of Medicine, University of Wisconsin-Madison, Madison, WI; [6]Geriatric Research, Education, and Clinical Center, William S. Middleton Memorial Veterans Hospital, Madison, WI; [7]Department 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 Carpentier[1]; Thibaud Godon[1, 2]; Maxime Deraspe[1]; Jacques Corbeil[1, 2]; *[1]Corbeil Laboratory, CRCHU de Quebec - Université Laval, Quebec, QC; [2]GRAIL, 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 Bouhaddou[1]; Ann-Kathrin Reuschl[2]; Benjamin Polacco[3]; Lucy G Thorne[2]; Manisha Ummadi[3]; Chengjin Ye[4]; Luis Martinez-Sobrido[4]; Lisa Miorin[5]; Kris White[5]; Danielle L Swaney[3]; Adolfo Garcia-Sastre[5]; Clare Jolly[6]; Lorena Zuliani-Alvarez[7]; Greg Towers[6]; Nevan J Krogan[3]; *[1]UCLA Mednet, Los Angeles, CA; [2]University College London, London, United Kingdom; [3]UCSF, San Francisco, CA; [4]Texas Biomedical Research Institute, San Antonio, Texas; [5]Icahn School of Medicine at Mount Sinai, New York, NY; [6]University College London, London, United Kingdom; [7]Novartis Institutes for Biomed.Research, Inc., Cambridge, MA*

WP 387 **A complete, modular, and flexible proteogenomic pipeline for peptide neoantigen discovery and verification**; Tyler Jubenville[1]; James E. Johnson[1]; Sue Rathe[1]; Flavia Popescu[1]; Kyle Richards[1]; Suzanne Coleman[1]; Reid Wagner[1]; Fengchao Yu[2]; Alexey I. Nesvizhskii[2]; Subina Mehta[1]; Pratik D Jagtap[1]; David Largaespada[1]; Timothy J. Griffin[1]; *[1]University of Minnesota, Minneapolis, MN; [2]University 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 Alves[1]; Aleksey Y Ogurtsov[1]; Roger Karlsson[2]; Daniel Jaen-Luchoro[2]; Beatriz Piñeiro-Iglesias[2]; Francisco Salvà-Serra[2]; Björn Andersson[2]; Edward R B Moore[2]; Yi-Kuo Yu[1]; *[1]CBB NCBI NLM NIH, Bethesda, MD; [2]University of Gothenburg, Gothenburg, Sweden*

WP 389 **Multi-omics data integration reveals clinical associated biomolecules in type 2 diabetes**; Xiaoyuan Zhou[1]; Alexey Stukalov[1]; Brittany Lee-McMullen[1]; Shadi Ferdosi[1]; Amir Alavi[1]; Guhan Venkataraman[1]; Harendra Guturu[1]; Anna Halama[2]; Frank Schmidt[2]; Karsten Suhre[2]; Daniel Hornburg[3]; *[1]Seer Inc., Redwood City, CA; [2]Weill Cornell Medicine - Qatar, Education City, Qatar; [3]Seer Inc, Redwood City, CA*

WP 390 **Leveraging the I.A.A Suite to Study the Impact of Drought in Sorghum and SetariaThrough Metabolomics GWAS and RNA-Seq**; Allen Hubbard[1]; Louis Connelly[1]; Shrikaar Kambhampati[2]; Collin Luebbert[1]; Hui Jiang[1]; Jennifer Barrett[1]; Madison Pope[1]; Xiaoping Li[1]; Ivan Baxter[1]; *[1]Donald Danforth Plant Science Center, Saint Louis, MO; [2]Salk Institute for Biological Sciences, La Jolla, California*

WP 391 **LinkedOmicsKB: A web portal for pan-cancer proteogenomics data analysis**; Sara R Savage[1]; Yuxing Liao[1]; Yongchao Dou[1]; Zhiao Shi[1]; Xinpei Yi[1]; Wen Jiang[1]; Jonathan T Lei[1]; Bing Zhang[1]; *[1]Baylor 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 Jaehnig[1]; Koi Pham[2]; Zhiao Shi[1]; Wen Jiang[1]; Sara R Savage[1]; Karsten Krug[3]; D. R. Mani[2]; Bing Zhang[1]; *[1]Baylor College of Medicine, Houston, Texas; [2]Broad Institute of MIT and Harvard, Cambridge, MA; [3]Frontier Medicines Corporation, Boston, MA*

WP 393 **Higher and higher N: SimpliFi data analysis for the masses now takes masses of samples**; Jim Palmeri[1]; John Wilson[1]; *[1]ProtiFi, LLC, Farmingdale, NY*

WP 395 **Multiomic Biomarkers in Livers of Streptozotocin-High Fat Diet Induced Non-Alcoholic Steatohepatitis (NASH) Mouse Model**; Ashok Panda[1]; Gayathree Karthikkeyan[1]; Daniel Domingo Fernández[1]; Venkata H. V Boddeda[1]; Virendra Chine[1]; Yogesh Aher[1]; Kundan Kumar[1]; Goutam Mondal[1]; Indranil Mukhopadhyay[1]; Biswapriya B. Misra[1]; Joe Rokicki[1]; Viswa Colluru[1]; *[1]Enveda Biosciences, Boulder, CO*

WP 396 **A Cloud-scalable Software Suite for Large-Scale Proteogenomics Data Analysis and Visualization**; Taylor Page[1]; Harsharn Auluck[1]; Margaret Donovan[1]; Aaron S Gajadhar[1]; Edwin Kwok[1]; Yuandan Lou[1]; Theo Platt[1]; Serafim Batzoglou[1]; *[1]Seer, 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 Zheng[1]; Martin Rendl[1]; Christopher

Pynn[1]; Ece Aydin[1]; Alec C Valenta[2]; Andrius Žilionis[3]; Robert Van Ling[4]; Wim Decrop[1]; Martin Samonig[1]; Anne Morgenstern[1]; *[1]Thermo Fisher Scientific, Germering, Germany; [2]Thermo Fisher Scientific, Somerset, NJ; [3]Thermo Fisher Scientific, Vilnius, Lithuania; [4]Thermo Fisher Scientific, Breda, Netherlands*

WP 398 **High-Resolution Separation of Bioisomers Using Ion Cloud Profiling Method**; Xiaoyu Zhou[1]; Zhuofan Wang[1]; Jingjin Fan[1]; Zheng Ouyang[1]; *[1]Tsinghua 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) Nikolaev[1]; Oleg Kharybin[1]; Gleb Vladimirov[1]; Sergey Gorbatov[1]; Anton Lioznov[1]; Petr Borisovets[1]; Alexander Semenov[1]; *[1]Skolkovo 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 Baek[1]; Chang Min Choi[2]; *[1]Korea Basic Science Institute, Cheongju, South Korea; [2]Korea Basic Science Institute, Cheoungju, South Korea*

WP 401 **Probing the First Stages of Photoinitiated Polymerisation with an On-Line Photochemical Reactor Coupled Mass Spectrometer**; Oisin J Shiels[1]; Maria Menti-Platten[2]; Brett Burns[2]; Paul Keller[2]; Philip J Barker[2]; Adam J Trevitt[2]; *[1]University of Wollongong, Wollongong, Australia; [2]University 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 Sugiyama[1]; Shun Kumano[1]; Yuichiro Hashimoto[2]; Akihiro Nojima[1]; *[1]Research & Development Group, Hitachi Ltd., Kokubunji-Shi, Japan; [2]Hitachi-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 Jordan[1]; Christian Lindinger[1]; Markus Müller[1]; Tobias Reinecke[1]; Markus Leiminger[1]; Klaus Winkler[1]; Lukas Märk[1]; Todd Rogers[2]; Philipp Sulzer[1]; *[1]IONICON Analytik GmbH., Innsbruck, Austria; [2]Trace VOC, Kennewick, WA*

WP 404 **An innovative prototype of mass spectrometry system based on a nano-opto-electromechanical (NOEMS) resonator sensor**; Wioletta Trzpil[1]; Adrien Reynaud[2]; Louis Dartiguelongue[3]; Vaitson Cumaku[3]; Guillaume Jourdan[1]; Sébastien Hentz[4]; Christophe Masselon[3]; Marc Sansa[1]; *[1]CEA-Leti, Université Grenoble Alpes, F-38000, Grenoble, France; [2]Oberon Sciences, 300 avenue des papeteries, Villard-Bonnot, France, Villard-Bonnot, France; [3]CEA, IRIG, Grenoble, France; [4]CEA, LITEN, Grenoble, France*

WP 405 **Development and hybridization of orthogonal acceleration ToFMS and QIT-ToF-SIMS**; Jaeyoing Eo[1]; Chang Min Choi[2]; *[1]Korea Basic Science Institute, Daejeon, South Korea; [2]Korea Basic Science Institute, Cheoungju, South Korea*

WP 406 **A Study of the Improved Limitations of Bicubic Interpolation for both Field Analysis and Trajectory Calculations in SIMION**; Robert Jackson[1]; Mark Osgood[1]; *[1]Ashwood Labs, LLC, Wilton, NH*

WP 407 **Characterization of a detection system with high sensitivity and dynamic range for a novel HRAM mass spectrometer**; Johannes Petzoldt[1]; Toby Shanley[1]; Wilko Balschun[1]; Philipp Cochems[1]; Bernd Hagedorn[1]; Christian Hock[1]; Barak Lavi[2]; Daniel Mourad[1]; Maximilian Ochmann[1]; Robert Ostermann[1]; Semyon Shofman[2]; Hamish Stewart[1]; Alexander Wagner[1]; Amit Weingarten[2]; Alexander A Makarov[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]El-Mul Technologies Ltd., Rehovot, Israel*

WP 408 **Versatile, long-lifetime, wide dynamic range detector for TOF applications**; Jonathan Garel[1]; Amit Weingarten[1]; Semyon Shofman[1]; Alexander Kadyshevitch[1]; *[1]El-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. Taylor[1]; Colin L Mackay[1]; *[1]University 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 Asef[1]; Facundo Fernandez[1]; *[1]Georgia 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 Rydberg[1]; Nicholas Manicke[1]; *[1]Indiana University Purdue University Indianapolis, Indianapolis, IN*

WP 412 **Development and Evaluation of a Novel Accumulation Ion Source for Chemically Instable Compounds**; Joshua Rieger[1]; Sanna Benter[1]; Markus Langner[1]; Niklas Pengemann[1]; Philippe Rotgänger[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University 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 Lies[1]; Haichuan Liu[2]; Takashi Baba[3]; Zoe Zhang[2]; Elliott Jones[2]; *[1]Sciex, Brea, CA; [2]SCIEX, Redwood city, CA; [3]SCIEX, Concord, ON*

WP 414 **LIFDI technique coupled to Orbitrap Exploris MS**; Mathias Linden[1]; Tobias P. Wörner[2]; Kerstin Strupat[2]; H. Bernhard Linden[1]; *[1]Linden CMS, Weyhe, Germany; [2]Thermo 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 Kafeenah[1]; Shu-Hui Chen[1]; *[1]National 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 Zhou[1]; Emir Nazdrajić[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON*

WP 417 **Automating Minimally-Invasive Liquid Microjunction Sampling to Profile Large, Intact Objects**; Hannah Amy Lawther[1]; G. Asher Newsome[1]; *[1]Smithsonian 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 Hatvany[1]; Emma-Le Olsen[1]; Elyssia S. Gallagher[1]; *[1]Baylor 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 Gehm[1]; Carolin Schwarz[2]; Sven Ehlert[3]; Denis Starostin-Penner[2, 3]; Johannes Passig[2]; Dominic Kastner[4]; Christian Menhard[4]; Eric Achterberg[5]; Andreas Walte[3]; Ralf Zimmermann[2]; *[1]Leibniz Institute for Baltic Sea Research, Rostock, Germany; [2]Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; [3]Photonion GmbH, Schwerin, Germany; [4]InnoLas Laser GmbH, Krailling, Germany; [5]GEOMAR 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. Olsen[1]; Jacob B. Hatvany[1]; Chih-Chieh Hsieh[2]; Craig A. Aspinwall[2]; Elyssia S. Gallagher[1]; *[1]Baylor University, Waco, TX; [2]University of Arizona, Tuscon, Arizona*

WP 422 **Electrochemically etched tapered-tip stainless-steel electrospray-ionization emitters**; Jordan T. Aerts[1]; Per E. Andren[1]; Erik T. Jansson[1]; *[1]Uppsala University, Uppsala, Sweden*

WP 423 **In-Situ Liquid Biopsy Combined with Native Surface Mass Spectrometry and Top-Down/Bottom-Up Proteomics**; Raul Villacob[1]; Sarah C Beno[1]; Neda Feizi Gilandeh[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

WP 424 **Direct Sampling and Ionization of E-Cigarette Aerosol**; Nicole C Auvil[1]; Mark E Bier[1]; *[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 Mahmoud[1]; Daniel D. Vallejo[1]; Facundo M Fernandez[1]; *[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 Benter[1]; Markus Langner[1]; Niklas Pengemann[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

WP 427 **In-tip microextraction enables fast profiling of phospholipid isomers in plasma by mass spectrometry**; Qiqian Zhang[1]; Penglong Lian[1]; Zheng Ouyang[1]; Wenpeng Zhang[1]; *[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 Hayes[1]; Blessing Egbejiogu[1]; Neda Feizi Gilandeh[2]; Kelcey B. Hines[1]; Touradj Solouki[2]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA; [2]Baylor University, Waco, TX*

WP 429 **High-Throughput 'Dip-n-Sip' OPI-MS/MS sampling**; Nate Hoxie[1]; Savannah Wood[1]; Vijay Veerisetty[1]; Anthony Garrison[1]; Pranav Bende[1]; John Janiszewski[1]; Jonathan Shrimp[1]; Colin Kelly[1]; Meghav Verma[1]; Charles Bonney[1]; Sam Michael[1]; Matthew Hall[1]; Peter Kovarik[2]; Chang Liu[2]; Thomas R. Covey[2]; *[1]NIH/NCATS, Rockville, MD; [2]SCIEX, Concord, ON*

WP 430 **Developing a low-cost general-purpose corporative multiport inlet for immediately accessible atmospheric pressure and vacuum ionization methods**; Charles N McEwen[1, 2]; Milan Pophristic[1]; *[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 Trimpin[1]; Trine Halvorsen[2]; James Wager-Miller[3]; Ken Mackie[3]; Milan Pophristic[4]; Charles McEwen[4]; Ellen Inutan[5]; *[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-Illigan Institute of Technology, Illigan City, Philippines*

WP 432 **Detection of plasma ions by coupling a high resolution TOF-MS at minimum distance to EUV-light focus point.**; Niklas Pengemann[1]; Adelind Elshani[2]; Ismael Gisch[2]; Hendrik Kersten[1]; Sascha Brose[2]; Carlo Holly[2]; Peter Gust[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany; [2]RWTH Aachen University, Aachen, Germany*

WP 433 **Structural characterization and identity confirmation of anthocyanins in plant extracts by direct injection ion mobility-mass spectrometry**; River Pachulicz[1]; Long Yu[2]; Blagojce Jovcevski[1]; Vincent Bulone[1, 2, 3]; Tara L Pukala[1]; *[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 Aderorho[1]; Christopher D. Chouinard[1]; *[1]Clemson University, Clemson, SC*

WP 435 **Differentiation of Regioisomers of Sulfobenzoic Acid by Traveling-wave Ion Mobility Mass Spectrometry (TW-IM-MS)**; Athula Attygalle[1]; Jinxin Zhang[1]; Meenu Kumar[1]; Spencer Pinto[1]; *[1]Stevens Institute of Technology, Hoboken, NJ*

WP 436 **Ion mobility tandem mass spectrometry of chondroitin sulfate disaccharide domains in biglycan**; Mirela Sarbu[1]; Raluca Ica[1]; Edie Sharon[2]; David E. Clemmer[2]; 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 Berthias[1]; Maša Babović[1]; Nurgül Bilgin[2]; Jasmin Mecinovic[2]; Ole Nørregaard Jensen[1]; *[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 Juliano[1]; Henry W Li[1]; Anna G Anders[1]; Zhuoer Xie[2]; Brandon T Ruotolo[1]; *[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 Shepard[1]; Jody C. May[1]; David M Hercules[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

WP 440 **Detection and Characterization of Bacteria in Surface Water using LC-IM-MS/MS**; Kimberly Y Kartowikromo[1]; Orobola E Olajide[1]; Ahmed M Hamid[1]; *[1]Auburn University, Auburn, AL*

WP 441 **Characterization of Diabetes Biomarkers using High Resolution Ion Mobility – Mass Spectrometry**; Michael W Christopher[1]; Daniel Debord[2]; Boone M. Prentice[1]; Richard A. Yost[1]; Timothy J. Garrett[1]; *[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 Gernold[1]; Joshua S. Wallace[1, 2]; Alicia Perez-Fuentetaja[3]; 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. Diamanti[1]; Reza Aalizadeh[1]; Dimitrios E. Damalas[1]; Georgios O. Gkotsis[1]; Bob Galvin[2]; Artem Filipenko[3]; Carsten Baessmann[4]; Nikolaos S. Thomaidis[1]; *[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 Wohlfahrt[1]; Emilee Mustor[1]; Jennifer Guergues[1]; Lindsey N Shaw[1]; Stanley Stevens Jr. [1]; *[1]University of South Florida, Tampa, FL*

WP 445 **Peptide collision cross section of 22 post-translational modifications**; Andreas Will[1]; Denys Oliinyk[1]; Florian Meier-Rosar[1]; *[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. Gkotsis[1]; Dimitrios E. Damalas[1]; Maria-Christina Nika[1]; Bob Galvin[2]; Carsten Baessmann[3]; Nikolaos S. Thomaidis[1]; *[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 Klein[1]; Komal Kedia[1]; Adam Sutton[1]; Jon Degnore[2]; Daniel Debord[2]; Xuanwen Shawn Li[1]; Hillary A. Schuessler[1]; *[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 Vallejo[1]; Vaclav Krupicka[2]; Aleksandra Popowich[3]; Julie Arslanoglu[3]; Caroline Tokarski[2]; Facundo M Fernandez[1]; *[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 Shestoperova[1]; Eric Strieter[1]; *[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. Miller[1]; Roman Manetsch[1]; Jared R. Auclair[1]; Jeffrey N. Agar[1]; *[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 Kaszycki[1]; Rory McCrimmon[1]; Ching Wu[1]; *[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 Rajkovic[1]; Maja Hammelrath[1]; Walter Wissdorf[1]; Thorsten Benter[1]; *[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 Schaefer[1]; Scott Hopkins[2]; Stefan Zimmermann[1]; *[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 Hammelrath[1]; Michelle Rajkovic[1]; Walter Wissdorf[1]; Thorsten Benter[1]; *[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 Deng[1]; Adam Engelson[1]; Miriam Fico[1]; Daniel Debord[1]; *[1]MOBILion Systems, Chadds Ford, PA*

WP 456 **Deep Ultraviolet Laser Ablation Electrospray Ionization for Native Mass Spectrometry**; Kelcey B. Hines[1]; Neda Gilandeh[2]; Raul Villacob[2]; Touradj Solouki[2]; Kermit K. Murray[1]; *[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. Makey[1]; Ryan Schroeder[1]; Keith Richardson[2]; David Langridge[2]; Jakub Ujma[2]; Kevin Giles[2]; Brandon T. Ruotolo[1]; *[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 Dearden[1]; Savannah R Porter[1]; 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 Rorrer[1]; Ryan Clingman[1]; Sidney Buttrill, Jr. [2]; Gordon A. Anderson[3]; Miriam Fico[1]; Daniel Debord[1]; *[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 Cropley[1]; Fanny C Liu[1]; Mengqi Chai[1]; Christian Bleiholder[1]; *[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. Brady[1]; Stacey Nash[1]; Kristalle G. Cruz[1]; Ishan V. Soni[1]; Jeanne A. Hardy[1]; Richard W. Vachet[1]; *[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 Lu[1]; Wenxin Wu[1]; Vu Ngoc Huong Tran[1]; Hua Zhang[1]; Min Ma[1]; Zhijun Zhu[1]; Shuling Xu[1]; Lingjun Li[1]; *[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. Williamson[1]; Gabe Nagy[1]; *[1]University of Utah, Salt Lake City, UT*

WP 464 **Regulations of Many Solution Structures of Chymotrypsin Inhibitor 2 though ESI-IMS-MS Measurements**; Hua Pan[1]; Shannon A. Raab[1]; Lucas W. Henderson[1]; Samantha R. Schrecke[2]; Arthur Laganowsky[2]; David H. Russell[2]; David E. Clemmer[1]; *[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 Moore[1]; Stacey Nash[1]; Richard W Vachet[1]; *[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. Edwards[1]; Anthony J. Blue[1]; Michael S. Cordes[1]; Jessica M. Conforti[1]; Michael A. Trakselis[1]; Elyssia S. Gallagher[1]; *[1]Baylor University, Waco, TX*

WP 467 **Composite Multidimensional Ion Mobility-Mass Spectrometry for Improved Differentiation of Stereochemical Modifications**; Xia Xu[1]; Li Han[1]; Zhen Zheng[2]; Rui Zhao[1]; Lingjun Li[3]; Xueguang Shao[1]; Gongyu Li[1]; *[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 Anders[1]; Brandon T Ruotolo[1]; *[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. Sharon[1]; Lucas W. Henderson[1]; Sarah M. O'keefe[1]; David E. Clemmer[1]; *[1]Indiana University Bloomington, Bloomington, IN*

WP 470 **Trapped ion mobility mass spectrometry in nucleic acid drug-discovery: revealing conformation-specific**

preferential binding to regulatory structures of the SARS-CoV-2 genome; Ghazaleh Yassaghi[1]; Thomas Kenderdine[1]; Jyotsna Kumar[1]; Daniele Fabris[1]; *[1]University 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 Wilson[1]; Holly Bohlin[1]; Susana Herrera[2]; Raphael Raptis[2]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN; [2]Florida International University, Miami, FL*

WP 472 **Correlating Conformation to Function of Disease-linked Labile Protein Surface Modifications UsingGlycoform-resolved Quantitative Unfolding Mass Spectrometry**; Yifei Jia[1]; Yamei Wang[1]; Gongyu Li[1]; *[1]Nankai University, Tianjin, China*

WP 473 **Predicting Collisional Cross Section at Ultra-High Precision Using Comprehensive Physics and Translational-Rotational Energy Partitioning**; Christopher Harrilal[1]; Sandilya V.B. Garimella[2]; Jaehun Chun[2]; Yehia M. Ibrahim[2]; Carlos Larriba-Andaluz[3]; Gregory K Schenter[2]; Richard D. Smith[2]; *[1]Pacific Northwest National Lab, Richland, WA; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Indiana 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 Siehl[1]; Alexis N. Edwards[1]; Elyssia S. Gallagher[1]; *[1]Baylor 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 Antle[1]; Sarah Dowd[2]; Diana Aga[1]; *[1]University at Buffalo, Buffalo, NY; [2]Waters 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 Hua[1]; Gandhi D Viraj[1, 2]; Carlos Larriba Andaluz[1]; *[1]IUPUI, Indianapolis, IN; [2]Purdue 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 Miller[1]; Kevin Jeanne Dit Fouque[1]; Fenfei Leng[1]; Francisco Alberto Fernandez Lima[1]; *[1]Florida International University, Miami, FL*

WP 479 **Distinguishing Photo crosslinked and non-Photo crosslinked Human Telomers by Ion Mobility Mass Spectrometry**; Hsin-Chieh Yang[1]; Savannah Scruggs[1]; Mengqi Chai[1]; John-Stephen Taylor[1]; Michael L. Gross[1]; *[1]washington university in St. Louis, saint louis, MO*

WP 480 **Thermal Stabilities of Disulfide-Reduced Lysozyme Conformations by Cyclic Ion Mobility-Mass Spectrometry**; Sarah O'keefe[1]; Lucas Henderson[2]; Edie M. Sharon[2]; David E. Clemmer[3]; *[1]Indiana University, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, Indiana; [3]Indiana 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 Yan[1]; Chuan-Fan Ding[2]; *[1]Ningbo University, Ningbo, China; [2]Ningbo University, Ningbo, China*

WP 482 **Trapped ion mobility separation (tims) of glucose -6 phosphate and fructose 6 phosphate**; Surendar Tadi[1]; Xuejun Peng[2]; Beixi Wang[3]; Erica Forsberg[4]; Matthew Lewis[5]; *[1]Bruker Daltonics, Billerica, MA; [2]Bruker Scientific, San Jose, CA; [3]Bruker Daltonics, San Jose, CA; [4]Bruker Scientific, LLC, Billerica, MA; [5]Bruker Dalton's GmbH & Co KG, Bremen, Germany*

WP 483 **Characterization of adeno-associated virus (AAV) capsid protein using microflow LC-MS/MS**; Lingsheng Chen[1]; Tie Gao[1]; Ji Luo[2]; Lihai Guo[1]; Xiang Li[3]; Hongxu Chen[1]; *[1]SCIEX, Beijing, China; [2]SCIEX, Shanghai, China; [3]Division 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 Suryawanshi[1]; Ashutosh Shelar[1]; Deepti Maheshwari[2]; Samruddha Chavan[1]; Nitin Shukla[1]; Nilesh Patil[1]; Purushottam Sutar[1]; Dr. Jitendra Kelkar[1]; Dr. Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [2]Spinco Biotech Pvt Ltd., Mumbai, India*

WP 485 **High-Throughput Quantification of Creatine Levels in Dried Blood Spot**; Keeley Jo Alexander[1]; Fiona Hubbard[2]; Frances Morris[2]; Kavinda Desilva[2]; Mariko Nakano, Phd[2]; Charles Sailey, Md[2]; Zane Hauck, Phd[2]; *[1]Molecular Testing Labs, Vancouver, WA; [2]Molecular 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 Pedersen[1]; Elizabeth Grose[1]; Andrew Horan[1]; Ashly Huber[1]; Joseph Worthington[1]; Alicia Broderick[2]; John Brady[2]; *[1]Signature Science, LLC, Egg Harbor Township, NJ; [2]Transportation Security Laboratory, Atlantic City, NJ*

WP 487 **Ultra-fast LC-MS Analyses using Short 10 mm Columns**; Matthew James[1]; Tony Edge[1]; David Dunthorne[1]; Mark Fever[1]; Katie Lawlor[2, 3]; Lewis Couchman[3]; Keng Tiong Ng[4]; Leon Barron[4]; Geoff Faden[5]; *[1]Avantor, Theale, United Kingdom; [2]Department of Analytical, Environmental and Forensic Sciences, King's College London, London, United Kingdom; [3]Analytical Services International, St. George's - University of London, London, United Kingdom; [4]Environmental Research Group, School of Public Health, Imperial College London, London, United Kingdom; [5]MAC-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 Spruill[1]; Ritu Bohat[2]; Howard Martin[3]; Weiyi Peng[2]; Xinli Liu[1]; *[1]Department of Pharmacological and Pharmaceutical Sciences, University of Houston, Houston, TX; [2]Department of Biology and Biochemistry, University of Houston, Houston, TX; [3]Sagis Diagnostics, Houston, TX*

WP 489 **Microflow 4D-Proteomics for robust, high-throughput sample analysis**; Florian Busch[1]; Andreas Schmidt[1]; Johanna Tüshaus[2]; Eike Mucha[1]; Thomas Kosinski[1]; Stephanie Kaspar-Schoenefeld[1]; Christoph Krisp[1]; Christoph Gebhardt[1]; Julie Munoz[1]; Jean-Francois Greisch[3]; Axel Maibaum[1]; Markus Lubeck[1]; Bernhard Küster[2]; Gary Kruppa[4]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]Chair of Proteomics and Bioanalytics, TUM, Freising, Germany; [3]Bruker Switzerland AG, Faellanden, Switzerland; [4]Bruker 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 Shukla[1]; Nitish Ramchandra Suryawanshi[1]; Purushottam Sutar[1]; Samruddha Chavan[1]; Nilesh Patil[1]; Dr. Jitendra Kelkar[1]; Dr. Pratap Rasam[1]; *[1]Shimadzu 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 Rasam[1]; Xiaoyu Zhu[2]; Timothy Sikorski[3]; Thomas Angel[3]; John T Mehl[3]; Jun Qu[1, 2]; *[1]Department of*

Biochemistry, State University of New York, Buffalo, NY; [2]Department of Pharmaceutical Sciences, State University of New York, Buffalo, NY; [3]GlaxoSmithKline, 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]; *[1]International Postgraduate School Jožef Stefan, Ljubljana, Slovenia; [2]Jožef Stefan Institute, Ljubljana, Slovenia; [3]Faculty of Pharmacy, University of Ljubljana, Ljubljana, Slovenia; [4]Department of Experimental Oncology, Institute of Oncology Ljubljana, Ljubljana, Slovenia; [5]Faculty of Health Sciences, Izola, Slovenia; [6]Faculty 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 Murisier[1]; Valentina D'Atri[1]; Vincent Larraillet[2]; Sebastian Pirner[2]; Miroslav Nikolov[2]; Davy Guillarme[1]; *[1]School of Pharmaceutical Sciences, Institute of Pharmaceutical Sciences of Western Switzerland, University of Geneva, Geneva, Switzerland; [2]Roche 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 Bu[1]; Woo Hyun Yoon[1]; Danielle Tonev[1]; Purvi Jejurkar[1]; *[1]Abbvie, South San Francisco, CA*

WP 495 **Analysis of Alkylphenol Ethoxylates (APEOs) and Alkylphenols (APs) in Textiles by UHPLC-MS/MS**; Jamie Foss[1]; Francisco A. Ferron[2]; Roberto Bozic[2]; *[1]PerkinElmer, Shelton, CT; [2]PerkinElmer, Milan, Italy*

WP 496 **Global metabolic profiling of E. Coli strains for producing soluble recombinant protein**; Meghna Srivastava[1]; Snehal Ganjave[2]; Deepti Sahastrabuddhe[2]; Vivek Mishra[3]; Prajval Nakrani[3]; Pramod P. Wangikar[2, 3]; *[1]Indian Institute of Technology, Bombay, Mumbai, India; [2]Indian Institute of Technology Bombay, Mumbai, India; [3]Clarity 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 Chaumier[1]; Clotilde Favino[1]; Charlotte Mappa[1]; Christine Albaret[1]; Emmanuel Joubert[1]; Anne Bossée[1]; *[1]DGA, Vert-Le-Petit, France*

WP 498 **Untargeted differential metabolomics of S. mutans biofilm on dental composites**; Chien-chia Chen[1]; Karabi Mondal[1]; Evan P. O'Brien[1]; Karl J. Rockne[1]; James L. Drummond[1]; Luke Hanley[1]; *[1]University of Illinois at Chicago, Chicago, IL*

WP 499 **Characterization of a Diverse Sample Collection by UPLC-MS**; Wilfredo Pinto[1]; Foster Tenkorang[1]; *[1]Merck, Rahway, NJ*

WP 500 **New Approach for Quantification and Measurement of Carbon Isotopes of Drugs with LC Coupled to FID and IRMS**; Herbert Tobias[1]; Andrew Jones[2]; Tommy Saunders[2]; J. Thomas Brenna[1]; *[1]University of Texas at Austin, Austin, TX; [2]Activated Research Company, Eden Prairie, MN*

WP 501 **Quantification of Psilocybin and Psilocin Content Variety in Psilocybe cubensis Strains with LC-MS**; Roman Goff[1]; Morgan Smith[1]; Jonathan Ferguson[2]; Kevin A. Schug[1]; Sue Sisley[3]; Paige Wicker[1]; *[1]University of Texas at Arlington, Arlington, TX; [2]Shimadzu Scientific Instrument, Columbia, MD; [3]Scottsdale 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 Palmer[1]; Aaron O Bailey[1]; William Russell[1]; *[1]University 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**; Žan Rekar[1, 2]; Agneta Annika Runkel[1]; Darja Mazej[1]; Tina Kosjek[1, 2]; Milena Horvat[1, 2]; *[1]Department of Environmental Sciences, Jožef Stefan Institute, Ljubljana, Slovenia; [2]International 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 Gibson[1]; Jingshu Guo[1]; Stephanie N. Samra[2]; *[1]Thermo Scientific, San Jose, CA; [2]Thermo 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 Bassett[1]; Luke Marney[2]; Jeffrey Morre[2]; Thando Mawasha[3]; Michael Harry[3]; Casey Kanalos[3]; Corey De La Cruz[4]; Daphne Guo[4]; Cheng Shi[4]; Lya Carini[4]; Kyle Barber[5]; Gerrad Jones[4]; Christine Kelly[3]; Tyler Radniecki[3]; Claudia Maier[2, 6]; *[1]Department of Biochemistry and Biophysics, Oregon State University, Corvallis, OR; [2]Department of Chemistry, Oregon State University, Corvallis, OR; [3]Chemical, Biological and Ecological Engineering, Oregon State University, Corvallis, OR; [4]Department of Biological and Ecological Engineering, Oregon State University, Corvallis, OR; [5]Athletics Integrity Unit, World Athletics, Monaco, Monaco; [6]Linus Pauling Institute, Oregon State University, Corvallis, OR*

WP 506 **Maximizing Sensitivity by Multifactorial Optimization of Method Parameters for Clinical Mass Spectrometry**; Evan W. McConnell[1]; Christopher M. Shuford[1]; Russell P. Grant[1]; *[1]Labcorp, 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 Sharif[1]; Sujit Biswas[1]; Michelle L Spruill[1]; Xinli Liu[1]; *[1]University of Houston, Houston, TX*

WP 508 **Chiral LC-MS/MS Methods for the Direct Separation and Analysis of Enantiomers to Understand Conversion in vitroand in vivo**; Yongjin Yao[1]; Bo Liu[1]; Wenchen Luo[1]; Cassandra Shu[1]; Danielle Tonev[1]; Purvi Jejurkar[1]; *[1]Abbvie, 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 Neale[1]; Alexandre Prefontaine[1]; Darien Yeung[1]; Victor Spicer[1]; Nediljko Budisa[1]; Helene Perreault[1]; Rene Zahedi[1]; Oleg V. Krokhin[1]; *[1]University of Manitoba, Winnipeg, MB*

WP 511 **Structural characterization of SARS-CoV-2 dimeric ORF9b reveals potential fold switching trigger mechanism**; Xiyue Jin[1]; Xue Sun[2]; Yan Chai[3]; Yu Bai[3]; Ying Li[3]; Tianjiao Hao[3]; Jianxun Qi[3]; Hao Song[3]; Catherine Cl Wong[4, 5, 6]; George Fu Gao[3]; *[1]University of Science and Technology of China, Heifei, China; [2]Peking University, Beijing, China; [3]Institute of Microbiology, Chinese Academy of Sciences, Beijing, China; [4]Peking University, Beijing, China; [5]Tsinghua-Peking University Joint Center for Life Sciences, Beijing, China; [6]Peking 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 Garza[1]; Genevieve James[1]; Hikyu Park[1]; Paul Baker[2]; J. Thomas Brenna[1]; *[1]University of Texas, Austin, TX; [2]SCIEX, Redwood city, CA*

WP 513 **Deep Profiling of Plasmalogens by Coupling the Paternò–Büchi Reactions with Tandem Mass Spectrometry**; Yichun Wang[1]; Yu Xia[1]; *[1]Tsinghua University, Beijing, China*

WP 514 **Assessment of multiple separation dimensions for confident annotation of novel microbial conjugated bile**

acids (MCBAs) using ion mobility spectrometry-mass spectrometry; James Dodds[1]; Allison K Stewart[2]; Emily C Gentry[3]; Matthew H Foley[4]; Lee R Hagey[5]; Pieter C Dorrestein[5]; Casey M Theriot[4]; Erin S Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Thermo Fisher Scientific, West Palm Beach, FL; [3]Virginia Tech, Blacksburg, VA; [4]North Carolina State University, Raleigh, NC; [5]University of California San Diego, San Diego, CA*

WP 515 **A method for comprehensive investigation of lipid ligands using LC-FRC/HRMS/MS**; Noriyuki Tomiyasu[1]; Yoshihiro Izumi[2]; Masatomo Takahashi[2]; Naoya Nishimura[3]; Kenji Toyonaga[3]; Sho Yamasaki[3]; Takeshi Bamba[2]; *[1]Kyushu University, Fukuoka, Japan; [2]Medical Institute of Bioregulation, Fukuoka, Japan; [3]Research 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 Jian[1]; Yu Xia[1]; *[1]Tsinghua University, Beijing, China*

WP 517 **Enhanced Annotation of Low-Abundant Lipid Species using Experimentally Generated Libraries**; Nicholas S Ly[1]; Jeremy K Chan[1]; Cunjie Zhang[1]; Andrew T Quaile[1]; Kelly Lozovschi[1]; Stephanie Z Xie[2]; J. Rafael Montenegro-Burke[1]; *[1]Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON; [2]Princess Margaret Cancer Centre, University Health Network, Toronto, ON*

WP 518 **Improving the performance of automated lipid identification for untargeted lipidomics**; William Xu[1]; Adriana Zardini Buzatto[1]; Elvis Lo[1]; Shuang Zhao[1]; Liang Li[1, 2]; *[1]The Metabolomics Innovation Centre (TMIC), Edmonton, AB; [2]University of Alberta, Edmonton, AB*

WP 519 **Comprehensive characterization of the lipid nanoparticle (LNP) ALC-0315 and its impurities using electron-activated dissociation (EAD)**; Zhichang Yang[1]; Sahana Mollah[2]; Paul Baker[1]; Robert Proos[3]; Jon Le Huray[4]; *[1]Sciex, Brea, CA; [2]SCIEX, Redwood City, CA; [3]Sciex, Framingham, MA; [4]Acuitas 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 Arao[1]; Yuta Miyazaki[1]; Hidenori Takahashi[1]; *[1]SHIMADZU Corporation, Kyoto, Japan*

WP 521 **The Caenorhabditis elegans lipidome blueprint – established using UHPLC- QTOF-MS and UHPLC-IMS-QTOF-MS**; Michael Tan[1]; Liesa Salzer[2]; Aiko Barsch[3]; Sven W. Meyer[3]; Stefanie Wernisch[3]; Matthew R. Lewis[3]; Michael Witting[1, 4]; *[1]Metabolomics and Proteomics Core, Helmholtz Munich, Neuherberg, Germany; [2]Research Unit Analytical BioGeoChemistry, Helmholtz Munich, Neuherberg, Germany; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]Chair 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. Ross[1]; Soumyadeep Sarkar[1]; Aivett Bilbao[1]; Joon-Yong Lee[1]; Daniel J Orton[1]; Josie G. Eder[1]; Meagan C. Burnet[1]; Richard D. Smith[1]; Jennifer E. Kyle[1]; Ernesto S. Nakayasu[1]; Xueyun Zheng[1]; *[1]Pacific 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 Rice[1]; Svitlana Liashenko[1]; Nathan Cassidy[1]; Peter B. O'Connor[1, 2]; *[1]Verdel Instruments Ltd, Camberley, United Kingdom; [2]University 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 Menzel[3]; Monica Liu[3]; Prabhu Rangabashyam[3]; Venkateswara R Narreddula[3]; Stephen J Blanksby[3]; Josef Cvačka[1, 2]; *[1]Institute of Organic Chemistry and Biochemistry of the CAS, Prague, Czech Republic; [2]Department of Analytical Chemistry, Faculty of Science, Charles University, Prague, Czech Republic; [3]School of Chemistry and Physics, Queensland University of Technology, Brisbane, Australia*

WP 525 **Gas-Phase Ion/Ion Strategy for the Differentiation of Isomeric Bis(monoacylglycero)phosphate and Phosphatidylglycerol Species by Shotgun Lipidomics**; De'shovon M. Shenault[1]; Caitlin E. Randolph[1]; Sarah T. Nsiah[1]; Scott A. McLuckey[1]; *[1]Purdue University, Lafayette, IN*

WP 526 **Tracking the metabolism of unsaturated fatty acids in Staphylococcus aureus using online Paternó-Büchi reactions**; Emily L Pruitt[1]; Libin Xu[1]; *[1]University of Washington, Seattle, WA*

WP 527 **High-Energy Collision-Induced Dissocation and In-source Decay MALDI of Metal-adducted Fatty acids**; Chioma J Akor; *The University of Alabama, Tuscaloosa, AL*

WP 528 **Lipid Nanoparticle Impurity Monitoring Using Single Quadrupole Mass Detection for Regulated Environments**; Duanduan Han[1]; Kellen Delaney[1]; Robert E. Birdsall[1]; Ying Qing Yu[1]; *[1]Waters Corporation, Milford, MA*

WP 529 **The atlas of brain glycosphingolipids revealed by selective enrichment and structural lipidotyping**; Zidan Wang[1]; Donghui Zhang[2]; Wenpeng Zhang[2]; Yu Xia[2]; *[1]Tsinghua university, Beijing, China; [2]Tsinghua University, Beijing, China*

WP 530 **Identification and Characterization of Impurities in Lipid Nanoparticle Components Using TOF-MS with In-silico Fragmentation Data Processing**; Kellen Delaney[1]; Duanduan Han[1]; Robert E. Birdsall[1]; Ying Qing Yu[1]; *[1]Waters 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 Mueller[1]; Gérard Hopfgartner[1]; *[1]University of Geneva, Geneva, Switzerland*

WP 532 **Resolve gut bacterial lipid isomerism by coupling mCPBA epoxidation with RPLC-MS/MS**; Kai-Li Chen[1]; Ting-Hao Kuo[1]; Cheng-Chih Hsu[1]; *[1]Department 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 Finn[1]; Wilthon Gilles[1]; Rayan Murtada[1]; Jinshan Gao[1]; *[1]Montclair 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. Reardon[1]; Katrina L. Leaptrot[1]; Jody C. May[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

WP 535 **Structural diversity of Leptospira lipid A: what can it reveal about pathogenesis?**; Helena Petrosova[1, 2]; Abanoub Mikhael[2]; Matthew Sherman[3]; Sophie Culos[1]; Alexandre Giraud-Gatineau[4]; Alloysius M. Gomez[1]; Robert K Ernst[3]; Caroline E. Cameron[1, 5]; Elsio A. Wunder Jr.[6]; Mathieu Picardeau[4]; David R Goodlett[1, 2]; *[1]University of Victoria, Victoria, BC; [2]University of Victoria Genome British Columbia Proteomics Center, Victoria, BC; [3]University of Maryland, Baltimore, MD; [4]Institut Pasteur, Paris, France; [5]University of Washington, Seattle, WA; [6]Yale School of Public Health, New Haven, CT*

WP 536 **Ozone-enabled fatty acid discovery reveals unexpected diversity in the human lipidome**; Jan Philipp Menzel[1]; Reuben S. E. Young[2]; Aurelie H. Benfield[3]; Julia S. Scott[4, 5]; Puttandon Wongsomboon[1]; Lukáš Cudlman[6, 7]; Josef Cvačka[6, 7]; Lisa M. Butler[4, 5]; Sonia T. Henriques[3]; Berwyck Poad[1]; Stephen J Blanksby[1]; *[1]School of Chemistry and Physics, Queensland University of Technology, Brisbane, Australia; [2]University of Wollongong, Wollongong, Australia;*

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WP 537 **A comparative study on the identification of plasma lipids using collision-induced dissociation and electron-activated dissociation**; Kiran Maan[1]; Dipankar Malakar[1]; Cagakan Ozbalci[2]; *[1]SCIEX, Bangalore, India; [2]SCIEX, Alderley Park, United Kingdom*

WP 538 **Detection and Characterization of Intact Oxidized Phospholipids Following Oxidative Insult of Immortalized Microglial Cells**; Yulemni Morel[1]; Nivedita Hegdekar[2]; Chinmoy Sarkar[2]; Marta Lipinski[2]; Jace W Jones[1]; *[1]University of Maryland, Baltimore School of Pharmacy, Baltimore, MD; [2]University of Maryland, Baltimore School of Medicine, Baltimore, Maryland*

WP 539 **Pathogenic Leptospira lipid A structural changes induced by growth conditions**; Sophie Culos[1]; Helena Petrosova[1, 2]; Abanoub Mikhael[1]; Alexandre Giraud-Gatineau[3]; Elsio A. Wunder Jr. [4]; Mathieu Picardeau[3]; David R Goodlett[1, 2]; *[1]UVic Genome BC Proteomics Centre, Victoria, BC; [2]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [3]Biology of Spirochetes Unit, Institut Pasteur, Paris, France; [4]Department 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 Wu[1]; Yikun Liu[1]; Wenpeng Zhang[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China*

WP 541 **Structure-centric annotation of phospholipids by Electron Activated Dissociation**; Vincen Wu[1]; Mario Povoa Correia[1]; Adriano Rutz[1]; Nicola Zamboni[1]; *[1]ETH Zurich, Zurich, Switzerland*

WP 542 **Activated Electron Photodetachment and Ultraviolet Photodissociation for Top-Down Characterization of Intact Bacterial Lipooligosaccharides**; James E Keener[1]; Jennifer S Brodbelt[1]; *[1]University 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 Vaňková[1]; Ondřej Peterka[1]; Jakub Idkowiak[1]; Robert Jirásko[1]; Beatrice Mohelníková Duchoňová[2]; Martin Loveček[2]; Bohuslav Melichar[2]; Michal Holčapek[1]; *[1]University of Pardubice, Pardubice, Czech Republic; [2]University 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 Man[1]; Dandan Si[2]; Zhimin Long[2]; *[1]sciex, beijing, China; [2]SCIEX, Beijing, China*

WP 546 **Comparison of Plasma Triacylglycerols and Cholesteryl Esters Measured via Supercritical Fluid Chromatography and Normal Phase LC-MS/MS**; Eunice A Grigorutsa[1]; Michael S Gardner[1]; Susan Kuklenyik[1]; John R Barr[1]; *[1]Centers for Disease Control and Prevention, Chamblee, GA*

WP 547 **Aziridination-Based13C-Isotope Labeled Tag for Lipid Accurate Relative Quantitation at the Isomer Level**; Hongyuan Yang[1]; Shuli Tang[1]; Syuan-Ting Kuo[1]; Xin Yan[1]; *[1]Texas 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. Lee[1]; Julie D. Saba[1]; Hui Zhao[2]; Yanan Yang[2]; *[1]Department of Pediatrics, Division of Hematology/Oncology, University of California-San Francisco, Oakland, CA; [2]Agilent 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 Romsdahl[1]; Jennifer J Linares[1]; William K Russell[1]; *[1]Mass 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 Yoo[1]; Duck-Hyun Kim[2]; Moonhee Park[2]; Kun Cho[1]; *[1]Korea Basic Science Institute, Ochang, South Korea; [2]Korea Basic Science Institute, Ochang, South Korea*

WP 551 **Development and Analytical Validation of a Sphingolipid Targeted Panel**; Crystal L. Pace[1]; Bradley C. Cochran[1]; Richard J. Robinson[1]; *[1]Metabolon, Morrisville, NC*

WP 552 **Robust UPLC-MRM-MS workflow that allows combined quantification of oxylipins and PUFAs in a single analysis**; Mona Khorani[1]; Liping Yang[1]; Jaewoo Choi[1, 2]; Lynne H. Shinto[3]; Claudia S. Maier[1, 2]; *[1]Department of Chemistry, Oregon State University, Corvallis, OR; [2]Linus Pauling Institute, Oregon State University, Corvallis, OR; [3]Department 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**; Ziying Xu[1]; Juan Pablo Palavisini[1, 2]; Sepideh Kiani Shabestari[3, 4]; Mathew Blurton-Jones[3, 4, 5]; Kevin F Bieniek[6]; Xianlin Han[1, 2]; *[1]Barshop Institute for Longevity and Aging Studies, University of Texas Health Science Center at San Antonio, San Antonio, Texas; [2]Department of Medicine, UT Health San Antonio, San Antonio, Texas; [3]Department of Neurobiology & Behavior, UC Irvine, Irvine, California; [4]Sue and Bill Gross Stem Cell Research Center, UC Irvine, Irvine, California; [5]4Institute for Memory Impairments and Neurological Disorders, UC Irvine, Irvine, California; [6]Department 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 Mostafa[1]; Julius Agongo[1]; Reagan McGuffee[1]; Scott Grady[1]; Christopher Arnatt[1]; David Ford[1]; James Edwards[1]; *[1]Saint Louis University, Saint Louis, MO*

WP 555 **UPC2-MS/MS for Quantitation of a Panel of Poly-unsaturated Fatty Acids and their Eicosanoid Oxylipin Metabolites**; Guille Metzler[1]; Carmen Fernandez-Metzler[1]; Richard C. King[1]; *[1]PharmaCadence Analytical Services, Hatfield, PA*

WP 556 **Lipid Mass Tags via Aziridination for Probing Unsaturated Lipid Isomers and Accurate Relative Quantification**; Tingyuan Yang[1]; Shuli Tang[1]; Syuan-Ting Kuo[1]; Dallas Freitas[1]; Madison Edwards[1]; Hongying Wang[1]; Yuxiang Sun[1]; Xin Yan[1]; *[1]Texas A&M University, College Station, TX*

WP 557 **Targeted 4D PASEF-based quantification strategy for clinical lipidomics**; Dhanwin Baker[1]; Raissa Lerner[2]; Laura Bindila[2]; *[1]University Medical Center of Mainz, Mainz, Germany; [2]University 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. Kamble[1]; Qibin Zhang[1, 2]; *[1]Center for Translational*

Biomedical Research, University of North Carolina at Greensboro, North Carolina Research Campus, Kannapolis, NC; [2]Department 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 Linares[1]; Trevor Romsdahl[1]; William Russell[1]; *[1]UTMB Health Mass Spectrometry Facility, Galveston, TX*

WP 561 **An automated LC-PB-MS workflow for large-scale analysis of lipid C=C isomers**; Nan Zhang[1]; Wenhui Pang[1]; Jiexun Bu[1]; Wenpeng Zhang[2]; Zheng Ouyang[2]; *[1]PURSPEC Technology (Beijing) Ltd., Beijing, China; [2]Tsinghua 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 Delkhosh[1]; Akeem Sanni[1]; Judith Nwaiwu[1]; Andrew I. Bennett[1]; Cristian D. Gutierrez-Reyes[1]; Yehia Mechref[1]; *[1]Texas 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 Chen[1]; Gopal Reddy Ramidi[1]; Syuan-Ting Kuo[1]; Dallas Freitas[1]; Luchen Wuyang[1]; Aidan Slagter[1]; Peiyu Cai[1]; Ashok Polu[1]; Xin Yan[1]; *[1]Texas A&M University, College Station, TX*

WP 564 **Targeted Lipidomic Analysis of Pediatric Leukemia Cells Using LC-MS/MS Triple Quadrupole**; Lihua Jiang[1]; Ruiqi Jian[1]; Tiffany Trinh[1]; Hui Zhao[2]; Yanan Yang[3]; Mark Sartain[3]; Maya Kasowski[4]; Michael Snyder[1]; *[1]Department of Genetics, Stanford University, Stanford, CA; [2]Agilent Technologies, Wilmington, DE; [3]Agilent Technologies, Santa Clara, CA; [4]School 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 Bailey[1]; Kari B Basso[2]; *[1]University of Florida, Gainesville, Florida; [2]University 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) Pham[1]; Raymond Thomas[2]; Lakshman W Galagedara[3]; *[1]Memorial University of Newfoundland, Corner Brook, NL; [2]Department of Biology, Faculty of Science, Western University, London, ON; [3]School 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 Pan[1]; Juan Pablo Palavicini[1]; Xinlin Han[1]; *[1]Barshop 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 Pourmand[1]; Kin Sing Lee[1]; James Pestka[1]; Jenifer Fenton[1]; Emily Somers[2]; Faith Strickland[2]; Tracy Fuller[2]; Angel Edwards[1]; Suzu Thompson[1]; *[1]Michigan State university, EAST LANSING; [2]University of Michigan-Ann Arbor, Ann Arbor, MI*

WP 569 **Metabolomics Evaluation of the Impact of Violet-Blue Light (405 nm) on Platelet Concentrate**; Jinchun Sun[1]; Neetu Dahiya[2]; Tom Schmitt[1]; Caitlin Stewart[3]; John Anderson[3]; Scott MacGregor[3]; Michelle MacLean[3]; Richard Beger[1]; Chintamani D. Atreya[2]; *[1]NCTR / USFDA, Jefferson, AR; [2]Office of Blood Research and Review, Center for Biologics Evaluation and Research, United States Food and Drug Administration, Silver Spring, MD; [3]The 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 Gao[1]; George Gonyea[1]; Keegan Orzechowski[1]; Alena La[1]; Nafees Norris[1]; Juan Aon[1]; Matthew Maust[1]; *[1]GSK, 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 Wells[1]; Refat Nimer[3]; Oliver Fiehn[1]; *[1]University of California, Davis, Davis, CA; [2]The University of Jordan, Amman, Jordan; [3]Jordan 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 Zambito[1]; Leanne Ohlund[1]; Nejia Lassoued[2]; Rodolphe Soret[2, 3]; Nicolas Pilon[2, 3]; Lekha Sleno[1, 3]; *[1]University of Quebec in Montreal (UQAM), Chemistry department, Montreal, QC; [2]University of Quebec in Montreal (UQAM), Biology Department, Montreal, QC; [3]CERMO-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 Barsch[1]; Patrick Groos[2]; Nikolas Kessler[2]; Matthias Szesny[2]; Sven W. Meyer[2]; Ilmari Krebs[2]; Heiko Neuweger[2]; Matthew R Lewis[2]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]Bruker 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 Quan[1]; Shuang Zhao[1, 2]; Liang Li[1, 2]; *[1]University of Alberta, Edmonton, AB; [2]The 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 Wang[1]; Wei Han[1]; Walter P. Maksymowych[2]; Liang Li[1, 3]; *[1]The Metabolomics Innovation Centre (TMIC), Edmonton, AB; [2]Canadian Research and Education (CaRE) Arthritis, Edmonton, AB; [3]Department 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]; *[1]University of Arkansas for Medical Sciences, Little Rock, AR; [2]Arkansas Children's Nutrition Center, Little Rock, AR*

WP 577 **A biological model of the ageing metabolome reveals potential clinically relevant biomarkers**; Domenica Berardi[1]; Emily G Armitage[2]; Simon Ashton[2]; Alan Barnes[2]; Neil Loftus[2]; Gillian Farrell[1]; Abdullah Al Sultan[1]; Ashley McCulloch[1]; David Watson[1]; Matthew Baker[3]; Zahra Rattray[1]; Nicholas JW Rattray[1]; *[1]Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, Glasgow, United Kingdom; [2]Shimadzu Corporation, Manchester, United Kingdom; [3]School 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 Speca[3]; Amandine Gerstenberg[1]; Aurore Tomezyk[1]; Mathieu Gaudin[1]; Rebecca Deprez-Poulain[2, 4]; David Launay[3]; Benoit Deprez[4]; Corinne Ramos[1, 2]; *[1]ImaBiotech, Loos, France; [2]CAPSTONE-ETN MSCA network, Lille, France; [3]Institute for Translational Research in Inflammation (INFINITE), U1286, Univ. Lille, Inserm, CHU Lille, Lille, France; [4]Drugs and Molecules for Living Systems, U1177, Univ. Lille, Inserm, Institut Pasteur de Lille, Lille, France*

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 Cope[2]; Dana L Carper[2]; Richard J Giannone[2]; Udaya C Kalluri[2]; Robert L Hettich[1, 2]; Paul Abraham[1, 2]; [1]*Graduate School of Genome Science and Technology, University of Tennessee, Knoxville, TN, USA, Knoxville, Tennessee;* [2]*Biosciences 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 Krakko[1]; Whitney L Stutts[1]; Madhavi Kakumanu[2]; Coby Schal[2]; [1]*Molecular Education, Technology and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC;* [2]*Department 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 Alfaez[1]; Bernadett Papp[2]; Timothy J. Garrett[3]; [1]*University of Florida, Gainesville, Florida;* [2]*University of Florida College of Dentistry, Gainesville, FL;* [3]*University of Florida, Gainesville, FL*

WP 582 **Application of Chemical Isotope Labelling LC-MS Metabolomics to Bovine Pregnancy Investigation**; Daniel Patience[1]; Shuang Zhao[1]; Marcos Colazo[2]; Graham Plastow[2]; Elda Dervishi[2]; Liang Li[1, 3]; [1]*The Metabolomics Innovation Centre (TMIC), Edmonton, AB;* [2]*Department of Agricultural, Food and Nutritional Science, University of Alberta, Edmonton, AB;* [3]*Department of Chemistry, University of Alberta, Edmonton, AB*

WP 583 **Iron Status in Early-Life Modulates Fecal Metabolomics in a Mouse Model**; Anastasiia Kostenko[1]; Hui Zhi[2]; Manuela Raffatellu[2]; Pieter C Dorrestein[3, 4]; Allegra T Aron[1]; [1]*Department of Chemistry and Biochemistry, University of Denver, Denver, CO;* [2]*Department of Pediatrics, University of California San Diego, La Jolla, CA;* [3]*Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA;* [4]*Collaborative 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 Radzikh[1]; Yana Sandlers[1]; [1]*Cleveland State University, Cleveland, OH*

WP 585 **Untargeted Urinary Metabolomic Profiling of Patients With Medium-Chain Acyl-Coenzyme A Dehydrogenase Deficiency**; Patrick T Stumps[1]; Pranoot Tanpaiboon[1]; Denise Z Salazar[1]; Scott M Goldman[1]; Nigel J Clarke[1]; [1]*Quest Diagnostics, San Juan Capistrano, CA*

WP 586 **Using linkage patterns to validate Internal Standard to natural-abundance Isotopic Envelope paired systems**; Chris Beecher[1]; Felice De Jong[1]; [1]*IROA Technologies, Chapel Hill, NC*

WP 587 **Untargeted metabolomics of Bombus impatiensshort-term responses to cold exposure via GC-MS**; Hunter Taylor[1]; Keaveny Ellen[1]; Michael Dillon[1]; Franco Basile[1]; [1]*University of Wyoming, Laramie, WY*

WP 588 **Serum Metabolomics and Lipidomics Studies to Identify Biomarkers for Hepatocellular Carcinoma**; Md Mamunur Rashid[1]; Rency S Varghese[1]; Habtom Ressom[1]; [1]*Georgetown University, Washington, DC*

WP 589 **Sexual Dimorphism of Rewarding System in Mouse Brain Revealed by Parallel Metabolomics and Lipidomics**; Huaxu Yu[1]; Tao Huan[1]; [1]*University of British Columbia, Vancouver, BC*

WP 590 **Tracing the origin of Chinese lotus root varieties using high-resolution mass spectrometry**; Jiao Liu[1]; Liuqing Zhao[2]; Jinmei Chen[2]; Zong Yang[2]; Bingjie Liu[3]; Lihai Guo[3]; [1]*Hubei Academy of Agricultural Sciences, Wuhan, China;* [2]*SCIEX, Shanghai, China;* [3]*SCIEX, Beijing, China*

WP 591 **Spatial metabolomics of polymicrobial wound infections and associated adhesive bandages**; Monica Ness[1]; Avery Holmes[2]; Laura-Isobel McCall[2, 3]; Carolyn Ibberson[2]; [1]*University of Oklahoma, Norman, OK;* [2]*University of Oklahoma, Department of Microbiology and Plant Biology, Norman, OK;* [3]*University 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. Corstvet[1]; Daniel D. Vallejo[1]; Molly E. Ogle[1]; Johnna S. Temenoff[1]; Facundo Fernandez[1]; [1]*Georgia 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 Wang[1]; Liang Li[1]; [1]*Department of Chemistry, University of Alberta, Edmonton, AB*

WP 594 **Developing Workflows to Effectively Probe the Cheese Rind Microbiome Metabolome**; Celine A Ertekin[1]; Laura Sanchez[1]; Gordon Luu[1]; [1]*University 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. Bellingeri[1]; Meng Li[1]; Yuko P. Y. Lam[1]; Christopher A. Wootton[2]; Mark P. Barrow[1]; Joanna F. Collingwood[1]; Peter B. O'Connor[1]; [1]*University of Warwick, Coventry, United Kingdom;* [2]*Bruker Dalton's GmbH & Co KG, Bremen, Germany*

WP 596 **CSF proteomic identification of disease-associated protein networks that distinguish between parkinsonian disorders**; Sophia Weiner[1]; Mathias Sauer[2]; Julius Constantinescu[3]; Radu Constantinescu[3]; Kaj Blennow[1, 2]; Henrik Zetterberg[1, 2, 4, 5, 6, 7]; Johan Gobom[1, 2]; [1]*Institute of Neuroscience and Physiology, Department of Psychiatry and Neurochemistry, University of Gothenburg, Mölndal, Sweden;* [2]*Clinical Neurochemistry Lab, Institute of Neuroscience and Physiology, Sahlgrenska University Hospital, Mölndal, Sweden;* [3]*Institute of Neuroscience and Physiology, Department of Neurology, the Sahlgrenska Academy at the University of Gothenburg, Gothenburg, Sweden;* [4]*Department of Neurodegenerative Disease, UCL Institute of Neurology, London, United Kingdom;* [5]*UK Dementia Research Institute, London, United Kingdom;* [6]*Hong Kong Center for Neurodegenerative Diseases, Hong Kong, China;* [7]*Wisconsin 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 Tognetti[1]; Yuehan Feng[1]; Roland Bruderer[1]; Dominique Kamber[1]; Jacqueline Darrow[2]; Alexandra Lewis[2]; Abhay Moghekar[2]; Lukas Reiter[1]; [1]*Biognosys AG, Schlieren, Switzerland;* [2]*Johns Hopkins University School of Medicine, Baltimore, MD*

WP 598 **Challenges in hypothesis building through multi-omics analysis of Alzheimer's disease plasma**; Yoshiya Oda[1]; Suzumi M Tokuoka[1]; Fumie Hamano[1]; Shumgo Adachi[2]; Tomohiro Andou[3]; Toru Natsume[2]; [1]*The University of Tokyo, Tokyo, Japan;* [2]*National Institute of Advanced Industrial Science and Technology, Tokyo, Japan;* [3]*Axcelead 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 Fonslow[1]; Bryan Boyd[1]; Nhi Ngo[1]; Rachel Herbst[1]; Jacquelyn Ha[1]; Tina Charlotte Stummann[2]; Micah Niphakis[1]; [1]*Lundbeck La Jolla Research Center, Inc., San Diego, CA;* [2]*H. Lundbeck A/S, Valby, Denmark*

WP 600 **Laser capture microdissection (LCM) enriched transcriptome and proteome differences between**

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 Olivares[1]; Carter Lantz[1]; Rachel R. Ogorzalek Loo[1]; Joseph A. Loo[1]; *[1]University 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 Hossain[1]; Francesca Rapino[1]; Dimitry Ofengeim[1]; Nellwyn Hagan[1]; Bailin Zhang[1]; Dhiman Ghosh[1]; *[1]Sanofi, Cambridge, MA*

WP 603 **Detection of epoxides and vicinal diols of docosahexaenoic acid in rat retinas by LC/MS/MS**; Genevieve E James[1]; Secilia Garza[1]; Hikyu Park[1, 2]; Paul Baker[3]; Mikhail Shchepinov[4]; J. Thomas Brenna[1, 2]; *[1]University of Texas at Austin, Austin, TX; [2]Dell Medical School, Department of Pediatrics, Austin, TX; [3]Sciex, Framingham, MA; [4]Biojiva, Los Altos, California*

WP 604 **Understanding Lipid Accumulation in and Around Amyloid Plaques Using Nano-DESI Mass Spectrometry Imaging**; Manxi Yang[1]; Emerson Hernly[1]; Palak Machanda[1]; Kaushik Sharma[1]; Connor Beveridge[1]; Mushfeqa Iqfath[1]; Matthew Muhoberac[1]; Gaurav Chopra[1]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN*

WP 605 **Characterization of brain O-glycosylation of mice with depressive-like behavior**; Youngsuk Seo[1]; Boyoung Lee[1]; *[1]Center 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. Randolph[1]; Palak Manchanda[1]; Connor Beveridge[1]; Kanchan Bisht[1]; Berwyck Poad[2]; Stephen J Blanksby[2]; Gaurav Chopra[1]; *[1]Purdue University, WEST LAFAYETTE, IN; [2]Queensland 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 Zemerov[1]; Lana Fabia[1]; Emma Gromacki[1]; Richard C. King[1]; Todd Herbst[2]; Celia Dominguez[2]; Edith Monteagudo[2]; Carmen Fernández-Metzler[1]; *[1]PharmaCadence Analytical Services, LLC, Hatfield, PA; [2]CHDI Foundation, Los Angeles, CA*

WP 608 **A Comparative Proteomic Analysis of Parkinson's Disease, Dementia with Lewy Bodies and Multiple Systems Atrophy**; Sinead Greally[1]; Mukesh Kumar[1]; Christoph N Schlaffner[1]; Sabina Berretta[2]; Hanno Steen[3]; Judith Steen[1]; *[1]Boston Children's Hospital, Boston, MA; [2]Harvard Brain Tissue Resource Center (HBTRC), McLean Hospital, Belmont, Boston, MA; [3]Boston 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 Ikegawa[1]; Soichiro Tokuhira[1]; Yumiko Toyama[1]; Takashi Nirasawa[2]; Masato Hoshino[3]; Motohiro Nishikawa[4]; Nobuto Kakuda[1]; Yuko Saito[5]; Shigeo Murayama[5]; *[1]Doshisha University, Kyotanabe City, Japan; [2]Bruker Japan K.K., Yokohama, Japan; [3]Japan Synchrotron Radiation Research Institute (JASRI/SPring-8), Harima, Japan; [4]Kyoto Institute of Nutrition & Pathology, Kyotanabe City, Japan; [5]Brain 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 Phetsanthad[1]; Elliot Patrenets[1]; Caroline Roycroft[1]; Hannah N. Miles[1]; Min Ma[1]; Pamela R. Westmark[1]; Cara J. Westmark[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 611 **A systematic method to quantify peptides in CSF for the analysis of neurodegenerative diseases**; Gennifer Merrihew[1]; Jea Park[1]; Deanna Plubell[1]; Julia E Robbins[1]; Brian C Searle[2]; Eric Huang[1]; Christine C. Wu[1]; Kathleen Poston[3]; Thomas J. Montine[3]; Michael J. MacCoss[1]; *[1]University of Washington, Seattle, WA; [2]Ohio State University, Columbus, OH; [3]Stanford University, Stanford, CA*

WP 612 **Identification of Spontaneous Chemical Modifications in Neurodegenerative Disease Brain Tissue**; Brielle L Van Orman[1]; Ibrar Siddique[2]; Gal Bitan[2]; Blaine Roberts[3]; Ryan R. Julian[1]; *[1]University of California, Riverside, Riverside, CA; [2]University of California, Los Angeles, Los Angeles, CA; [3]Emory University, Atlanta, GA*

WP 613 **Tissue Specific Interactome of the NPC1 Cholesterol Transporter**; Roshan Javanshad[1]; Thu T. A. Nguyen[1]; Stephanie M Cologna[1]; *[1]University of Illinois at Chicago, Chicago, IL*

WP 614 **Spatiotemporal Proteomics of Human iPSC-derived Neuron Model of Frontotemporal Dementia**; Wan Nur Atiqah Mazli[1]; Jiawei Ni[1]; Ashley Frankenfield[1]; Ling Hao[1]; *[1]Department 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 Chu[1]; Huan Sun[1]; Yun Jiao[1]; Junmin Peng[1]; *[1]Stjude 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 Morgenstern[1]; Hila Levy[2]; Nili Tickoysky[3, 4]; Lei Yu[5]; Aron S. Buchman[5]; David A. Bennet[5]; Michal Schneider Beeri[3, 6]; Yishai Levin[2]; *[1]Weizmann Institute, Rehovot, Israel; [2]Weizmann Institute of Science, Rehovot, Israel; [3]The Joseph Sagol Neuroscience Center, Sheba Medical Center, Ramat Gan, Israel; [4]The Goodman faculty of life sciences, Bar Ilan University, Ramat Gan, Israel; [5]Rush Alzheimer's Disease Center, Rush University, Chicago, IL; [6]Icahn 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. Greco[1]; Joshua L Justice[1]; Josiah E Hutton[1]; Tavis J Reed[1]; Jeffrey P Cantle[2]; Michelle A Kennedy[1]; Bokai Song[1]; Alma M Perez[3, 4]; Ismael Al-Ramahi[3, 4]; Juan Botas[3, 4]; Jeffrey B Carroll[5]; Ileana M Cristea[1]; *[1]Princeton University, Princeton, NJ; [2]Western Washington University, Department of Psychology, Bellingham, WA; [3]Jan and Dan Duncan Neurological Research Institute, Houston, TX; [4]Baylor College of Medicine, Department of Molecular and Human Genetics, Houston, TX; [5]University 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 Chen[1]; Xiaomei He[1]; Yen-Yu Yang[1]; Yinsheng Wang[1]; *[1]University 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 Guo[1]; Trishika Chowdhury[1]; Walter P. Galie[1]; Kellye A. Cupp-Sutton[1]; Dahang Yu[1]; Si Wu[1]; *[1]University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK*

WP 620 **Analysis of the Δhnox Caulobacter crescentus proteome and c-di-GMP pools using LC-MS**; Cameron C Lee-Lopez[1]; Md. Shariful Islam[1]; Erik T Yukl[1]; *[1]New Mexico State University, Las Cruces, NM*

WP 621 **Long-term quantitative and qualitative reproducibility of capillary zone electrophoresis-tandem mass spectrometry for top-down proteomics of complex proteome samples**; Amirhossein Sadeghi[1]; Qianyi Wang[1]; Wenrong Chen[2]; Xiaowen Kevin Liu[3]; Liangliang Sun[1]; *[1]Michigan State university, EAST LANSING; [2]Indiana University Purdue University Indianapolis, Indianapolis, IN; [3]Tulane 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 Ali[1]; Karim Aljakouch[1, 2]; Jeroen Krijgsveld[1, 2]; *[1]German Cancer Research Center, Heidelberg, Germany; [2]Heidelberg University, Heidelberg, Germany*

WP 623 **Exploring RNA Binding Interactome in Mouse Macrophages**; Matthew J Marino[1]; Deepali Rathore[2]; Aleksandra Nita-Lazar[2]; *[1]National Institute of Health, Bethesda, MD; [2]NIH/NIAID, Bethesda, MD*

WP 624 **Label-Free Quantitation of Protein Mixtures using Data-Independent Acquisition (DIA)**; Randy J Arnold[1]; Takeshi Shibata[2]; Ushio Takeda[2]; Haruka Kumabe[3]; Takeshi Masuda[3]; Sumio Ohtsuki[3]; Patrick Pribil[4]; *[1]SCIEX, Bloomington, IN; [2]K. K. AB SCIEX, Tokyo, Japan; [3]Kumamoto University, Kumamoto, Japan; [4]SCIEX, Concord, ON*

WP 625 **QCQuan: a new tool for rapid quality assessment of quantitative proteomics experiments**; Simon Appeltans[1]; Joris Van Houtven[1]; Jef Hooyberghs[1]; Dirk Valkenborg[1]; *[1]Hasselt 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. Martins[1]; Livia Luz[2]; Diego Assis[3]; Daniel B. McClatchy[1]; Jolene K. Diedrich[1]; Alysson Muotri[2]; John Robert Yates III[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Sanford Consortium for Regenerative Medicine, UCSD, San Diego, CA; [3]Bruker Daltonics, San Jose, CA*

WP 627 **A complementary ion-based strategy enables multiplexed quantification in ETD analysis using DiLeu isobaric tags**; Ting-Jia Gu[1]; Peng-Kai Liu[2]; Danqing Wang[3]; Zichong Li[4]; Lingjun Li[1, 2, 3]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Biophysics Program, University of Wisconsin–Madison, Madison, WI; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [4]University 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 Kwan[1]; Stephanie Lee[1]; Gina De Boer[1]; Janette Mezeyova[1]; Richard Dean[1]; Shohei Iwamoto[2]; Luis Sojo[1]; *[1]Xenon Pharmaceuticals, Burnaby, BC; [2]University 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 Bashyal[1]; Mukesh K. Venkat Ramani[2]; Yan Zhang[2]; Jennifer S. Brodbelt[1]; *[1]Department of Chemistry, The University of Texas at Austin, Austin, TX; [2]Department of Molecular Biosciences, The University of Texas at Austin, Austin, TX*

WP 630 **Proteomics and honey bee health**; Renata Moravcova[1]; Kyung-Mee Moon[1]; Greg R. Stacey[1]; Jason C. Rogalski[2]; Xiaojing Yuan[2]; Stephen F. Pernal[3]; Marta M Guarna[3]; Shelley Hoover[4]; Ida M. Conflitti[5]; Amro Zayed[5]; Robert Currie[6]; Pierre Giovenazzo[7]; Mateus Pepinelli[5]; Leonard J. Foster[1]; *[1]Department of Biochemistry and Molecular Biology, UBC, Vancouver, BC; [2]Proteomics Core Facility, UBC, Vancouver, BC; [3]Agriculture and Agri-Food Canada, Beaverlodge, AB; [4]Department of Biological Sciences, University of Lethbridge, Lethbridge, AB; [5]Department of Biology, York University, Toronto, ON; [6]Department of Entomology, University of Manitoba, Winnipeg, MB; [7]Département 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. Hughes[1]; Martin E. Palmer[1]; James I. Langridge[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

WP 632 **Accurate and precise label-free quantification with comprehensive proteome coverage using a novel HRAM platform**; Zilu Ye[1]; Anna Pashkova[2]; Ulises H. Guzmán[1]; Florian Harking[1]; Tabiwang N. Arrey[2]; Hamish Stewart[2]; Ana Martinez Del Val[1]; Yue Xuan[2]; Eugen Damoc[2]; Jesper V. Olsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, Copenhagen, Denmark; [2]Thermo 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 Aragon[1]; Valdemaras Petrosius[1]; Tabiwang N. Arrey[2]; Nil Üresin[3]; Benjamin Furtwängler[3]; Bo Porse[3]; Hamish Stewart[2]; Nicolaie Eugen Damoc[2]; Vlad Zabrouskov[2]; Erwin M. Schoof[1]; *[1]Technical University of Denmark, Kgs. Lyngby, Denmark; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]BRIC - University of Copenhagen, København, Denmark*

WP 634 **Surfaceome characterization in development of CAR-T therapies**; Ruzena Filandrova[1, 2]; Pauline Douglas[1, 2]; Xueyang Guo[2]; Theodore B. Verhey[1, 2]; Sorana Morissy[1, 2]; David C Schriemer[1, 2]; *[1]Department of Biochemistry and Molecular Biology, University of Calgary, Calgary, AB; [2]Arnie 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 Johnson[1]; Jingjing Huang[2]; William D. Barshop[2]; Jesse D. Canterbury[2]; Vlad Zabrouskov[2]; Graeme McAlister[2]; Martin Wühr[1]; *[1]Princeton University, Princeton, NJ; [2]Thermo Fisher Scientific, San Jose, California*

WP 636 **Quaternary amine tags for improved complement-quantitation in proteomics samples**; Nick Brodie[1]; David C Schriemer[1]; *[1]University 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 Jackson[1]; Shanyan Chen[1]; Martin Langenderfer[2]; Chao Li[1]; Heather R. Siedhoff[1]; Ashley Balderrama[1]; Runting Li[1]; Catherine E. Johnson[2]; C. Michael Greenlief[1]; Ibolja Cernak[3]; Ralph G Depalma[4]; Jiankun Cui[1]; Zezong Gu[5]; *[1]University of Missouri-Columbia, Columbia, MO; [2]Missouri University of Science and Technology, Rolla, MO; [3]Mercer University, Columbus, GA; [4]Department of Veterans Affairs, Washington DC, DC; [5]University of Missouri, Columbia, MO*

WP 638 **Functionalized Nanoparticles Enable Quantitative and Precise Large-Scale Unbiased, Deep Plasma Proteomics**; Ting Huang[1]; Jian Wang[1]; Alexey Stukalov[1]; Margaret Donovan[1]; Shadi Ferdosi[1]; Lucy Williamson[1]; Seth Just[1]; Gabriel Castro[1]; Eltaher Elgierari[1]; Ryan Benz[1]; Yingxiang Huang[1]; Khatereh Motamedchaboki[1]; Omid C. Farokhzad[1]; Serafim Batzoglou[1]; Simion Kreimer[2]; Asim Siddiqui[1]; Jennifer E. Van Eyk[2]; Daniel Hornburg[1]; *[1]Seer, Inc., Redwood City, CA; [2]Cedars-Sinai Medical Center, Los Angeles, CA*

WP 639 **Developing Cell Quenching Method to Facilitate Single Cell Mass Spectrometry Metabolomics Studies**; Deepti Bhusal[1]; Shakya Sankalpani Gunasena Wije Munige[1]; Zongkai Peng[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK*

WP 640 **Single-Cell Proteomic Analysis of Drosophila Oocytes**; Merin M. Rixen[1]; Rachel R. Ogorzalek Loo[1]; Joseph A. Loo[1]; Margot E. Quinlan[1]; *[1]UCLA, Los Angeles, CA*

WP 641 **Evaluation of sample preparation methods for single cell MALDI-MS**; Stanislav S. Rubakhin[1, 2]; Jonathan V.

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 Truong[1]; Madisyn Johnston[1]; Kei Webber[1]; Hannah Boekweg[1]; Caleb Lindgren[1]; Yiran Liang[1]; Alissia Nydeggar[1]; Xiaofeng Xie[1]; Samuel H Payne[1]; Ryan Kelly[1]; [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 Ebrahimi[1]; Stanislau Stanisheuski[1]; Liping Yang[1]; Luke C. Marney[1]; Kavi Aashish Vaidya[1]; Claudia Maier[1]; [1]*Oregon State University, Corvallis, OR*

WP 644 **Improving accuracy of protein quantitation in single-cell proteomics**; Connor A Peterson[1]; Hannah Boekweg[1]; Samuel H Payne[1]; [1]*Brigham Young University, Provo, UT*

WP 645 **Improving throughput of Single Cell Analysis through Hyperplexing and PairQuant Acquisition with inSeqAPI**; Tommy K. Cheung[1]; Hanna G Budayeva[2]; Ying Zhu[1]; Christopher M Rose[1]; [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**; Stanislau Stanisheuski[1]; Hyo Sang Jang[2]; Liping Yang[1]; Jeffrey Morre[1]; Claudia Maier[1]; [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 Matzinger[1]; Rupert L. Mayer[1]; Karl Mechtler[1]; [1]*Protein Chemistry Group, IMP, Vienna, Austria*

WP 648 **High-throughput nano LC-MS for sample-limited proteomics**; Alec C Valenta[1]; Christopher Pynn[2]; Dominic Hoch[3]; Manuel Matzinger[4]; Rupert L. Mayer[4]; Alexander Makarov[5]; Karl Mechtler[4]; Runsheng Zheng[2]; [1]*Thermo Fisher Scientific, Somerset, NJ;* [2]*Thermo Fisher Scientific, Germering, 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 Vu[1]; Carlos Eduardo Rodriguez-Lopez[2]; Delia Ayled Serna Guerrero[2]; Sarah Ellen O'Connor[1]; Lorenzo Caputi[1]; [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 Senavirathna[1]; Cheng Ma[1]; Ru Chen[2]; Sheng Pan[1]; [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 Ali[1]; 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 Petrosius[1]; Tabiwang N. Arrey[2]; Hamish Stewart[2]; Nicolaie Eugen Damoc[2]; Vlad Zabrouskov[3]; Erwin M. Schoof[1]; [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 Gao[1]; Anne-Lise Marie[1]; Alexander R. Ivanov[1]; [1]*Northeastern University, Boston, MA*

WP 654 **Automated Single-Cell Metabolomics to Map Molecular Transducers of MSC Senescence**; Joseph L. Corstvet[1]; Samuel M. Ehrlich[1]; Daniel D. Vallejo[1]; Molly E. Ogle[1]; Bo Yang[1]; Alexandra E. Dunnum[1]; Mohamed W. Badawy[1]; Johnna S. Temenoff[1]; Craig R. Forest[1]; Facundo Fernandez[1]; [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 Krisp[1]; Dorte Bekker-Jensen[2]; David Hartlmayr[3]; Anjali Seth[3]; Moritz Heusel[2]; Magnus Huusfeldt[2]; Thorsten Ledertheil[1]; Jean-Francois Greisch[1]; Andreia Almeida[4]; Jarrod Sandow[4]; Guilhem Tourniaire[3]; Nicolai Bache[2]; Markus Lubeck[1]; Gary Kruppa[5]; [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-Jensen[1]; Christoph Krisp[2]; David Hartlmayr[3]; Anjali Seth[3]; Ole B. Hoerning[1]; Moritz Heusel[1]; Magnus Huusfeldt[1]; Andreia Almeida[4]; Jarrod Sandow[4]; Markus Lubeck[2]; Gary Kruppa[5]; Nicolai Bache[1]; [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 Boekweg[1]; Samuel H Payne[1]; [1]*Brigham Young University, Provo, UT*

WP 658 **Metabolomic coverage of small cell populations**; Julius Agongo[1]; James Edwards[1]; [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 Galie[1]; Zhitao Zhao[1]; Trishika Chowdhury[1]; Samin Anjum[1]; Yanting Guo[1]; Kellye A Cupp-Sutton[1]; Si Wu[1]; [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 Fulcher[1]; Lye Meng Markille[2]; Hugh D Mitchell[2]; Sarah M Williams[2]; Kristin M Engbrecht[3]; Ronald J Moore[4]; William Chrisler[4]; Joshua Cantlon-Bruce[5]; Johannes W Bagnoli[5]; Anjali Seth[5]; Ljiljana Paša-Tolić[2]; Ying Zhu[2]; [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 Nitz[1]; Jose Humberto Giraldez Chavez[1]; Samuel H Payne[1]; [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 Ortiz[1]; Ricardo dos Reis Silvestre[2]; Natalia Gasilova[1]; Rémi Martinent[2]; Cyril Portmann[2]; Luc Patiny[1]; Vincent Mutel[3]; Laure Menin[1]; [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 Zhang[1]; Wenxin Wu[1]; Lingjun Li[1]; [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 Awad[1]; Ana

Celia Grenier Ph.d[1]; Lawrence J. Andrade[1]; *[1]Dominion Diagnostics, North Kingstown, RI*

WP 665 **Removal Of Potential Pitfalls- Improve Ruggedness of Bioanalytical Method by Focusing On Assay Details**; Xiaodong Zhu[1]; Jingguo Hou[1]; Perry Fan[1]; Andrew Cunningham[1]; *[1]Worldwide Clinical Trials, Austin, TX*

WP 666 **Mass Spectrometry-guided Synthesis of Iodoacetyl Black Hole Quenchers**; Pradnya Patil[1]; Karine Bagramyan[1]; Daniel Röth[1]; Markus Kalkum[1]; *[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 Gachumi[1]; Aimee Schryer[1]; Steven Siciliano[1]; *[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 Lu[1]; Chia-Yi Kuan[2]; Siming Wang[1]; *[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 Kang[1]; Yoondam Seo[1]; Hyeon-Jeong Lee[1]; Junghyun Son[1]; Hophil Min[1]; *[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 Balcer[1]; Yelena Adelfinskaya[1]; Chris J Brown[1]; Mike Madary[1]; Jeffrey R Gilbert[1]; Suresh Annangudi[1]; *[1]Corteva Agriscience, Indianapolis, IN*

WP 671 **Prioritization Strategies for Non-Target Screening and Applications to Recycled Textile Analysis of Emerging Contaminants**; Drew Szabo[1]; Varvara Apostolopoulou Kalkavoura[1]; Aji Mathew[1]; Anneli Kruve[1]; *[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-Mairinger[1]; Sven Kochmann[1, 2]; Tim J. Causon[1]; Stephan Hann[1]; *[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 Hackett[1]; Lawrence J. Andrade[1]; Ana Celia Grenier Ph.d[1]; Amber Awad[1]; *[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 Ghosh[1]; Michael L Neugent[2]; Karsten Liegmann[3]; Brian Shofran[3]; Nicole J. De Nisco[2]; Vladimir Shulaev[1]; *[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 Jellick[1]; Kim Lohmeyer[2]; Dee Ellis[3]; Stephan BH Bach[1]; *[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 Alonso[1]; Nick Jones[1]; Joseph E Binkley[1]; *[1]Leco Corporation, St. Joseph, MI*

WP 678 **Bioanalysis of hydroxyl-dendrimer therapeutics using LC-MS/MS with in-source fragmentation**; Jason S Watts[1]; Emily Taylor[1]; Natacha Le Moan[2]; Jeff Cleland[2]; Jennifer Zimmer[1]; *[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 Bouchibti[1]; Cathy Chen[2]; Carlito B. Lebrilla[2]; *[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. Perez[1]; John J. Thaden[1]; Gabriella A.M. Ten Have[1]; Nicolaas E.P. Deutz[1]; *[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**; Nilesh Patil[1]; Ashutosh Shelar[1]; Samruddha Chavan[1]; Nitish Ramchandra Suryawanshi[1]; Nitin Shukla[1]; Purushottam Sutar[1]; Dr. Jitendra Kelkar[1]; Dr. Pratap Rasam[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

WP 682 **Elucidating Gut Microbial Metabolism with Mass Spectrometry Through 13C Labeled Dietary Fiber**; Christopher Suarez[1]; Cheng-Yu Weng[1]; Chad Masarweh[1]; David Mills[1]; Carlito Lebrilla[1]; *[1]University of California, Davis, Davis, CA*

WP 683 **AQMID-MS determines histone methylation with methyl donors from different metabolic sources**; Hui Tang[1]; Mark Sowers[1]; Kangling Zhang[1]; *[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. Rensner[1]; Paul Lueth[1]; Bryan Bellaire[1]; Young Jin Lee[1]; *[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 Zhang[1]; Brian C Sanders[1]; Hugh M O'Neill[1]; 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 Dias[1]; Darby Ball[1]; Oladimeji S Olaluwoye[1]; Javier Flores[1]; Sheena D'arcy[1]; *[1]University of Texas at Dallas, Richardson, TX*

WP 688 **Discovery of metabolic signature in hepatic fibrosis and pulmonary fibrosis using 13C-MFA**; Mijeong Kim[1]; Hyun Ju Yoo[1]; *[1]Asan medical center, Seoul, South Korea*

WP 689 **A New Set of Isobaric Labeling Reagents for Quantitative 16-Plex Proteomics**; Xiaolian Ning[1]; Qidan Li[2]; Jin Zi[2]; Zhanlong Mei[2]; Jie Liu[2]; Yuxing Zhang[2]; Mao Bi[3]; Xingang Liu[4]; Chao Lv[4]; Hequan Yao[5]; Jianguo Sun[5]; Feng Rao[3]; Shuwei Li[4, 5]; Siqi Liu[2]; *[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 Wang[1]; Ethan Stancliffe[1]; Michaela Schwaiger-Haber[1]; Leah P. Shriver[1]; Gary J. Patti[1]; *[1]washington university in St. Louis, saint louis, MO*

WP 691 **Profiling the human urinary proteome using a dimethyl-based multiplex-DIA workflow**; Ericka Itang[1]; Marvin

Thielert[1]; Johannes Müller-Reif[1, 2]; Vincent Albrecht[1]; Martin Steger[3]; Matthias Mann[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]OmicEra Diagnostics GmbH, Planegg, Germany; [3]NEOsphere Biotechnologies GmbH, Planegg, Germany*

WP 692 **Data-driven approach to resolve precursor enrichment in metabolic labeling**; Henock M. Deberneh[1]; Justin Zhu[1]; Rovshan G. Sadygov[1]; *[1]University of Texas medical branch, Galveston, TX*

WP 693 **Quantifying Protein Synthesis Using Orbitrap Gas Chromatography High-resolution Mass Spectrometry**; Xiaorong Fu[1]; Stanisław Deja[2]; Justin Fletcher[1]; Jeffrey Browning[1]; Shawn Burgess[1]; *[1]UT Southwestern Medical Center, Dallas, TX; [2]UT Southwestern Medical Center, dallas, Texas*

WP 694 **Dual tagging for multiplex quantitative metabolomics using LC-HRMS**; Briana Mwinkom Tengan[1]; James Edwards[1]; Micheal Armbruster[1]; *[1]Saint 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-Diz[5]; Maya Aleksandrova[5]; Yetis Gultekin[6, 7]; Argit Marishta[2, 4]; Lin Wang[1, 2]; Lifeng Yang[1, 2]; Shawn Davidson[2]; Martin Wuehr[1, 4]; Matthew G Vander Heiden[6, 7]; Daniel Herranz[5]; Jessie Yanxiang Guo[5]; Yibin Kang[3, 4]; Joshua D Rabinowitz[1, 2, 3]; *[1]Department of Chemistry, Princeton University, Princeton, NJ; [2]Lewis-Sigler Institute for Integrative Genomics, Princeton University, Princeton, NJ; [3]Ludwig Institute for Cancer Research, Princeton University, Princeton, NJ; [4]Department of Molecular Biology, Princeton University, Princeton, NJ; [5]Cancer Institute of New Jersey, Rutgers University, New Brunswick, NJ; [6]6. Koch Institute for Integrative Cancer Research, Massachusetts Institute of Technology, Boston, MA; [7]Department 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 Rahman[1]; A D A Shahinuzzaman[1]; Abu Hena Mostafa Kamal[2]; Saiful Chowdhury[1]; *[1]University of Texas at Arlington, Arlington, TX; [2]Baylor College of Medicine, Houston, TX*

WP 697 **MitoMap – A three-dimensional landscape of mitochondrial architecture**; Kerem Can Akkaya[1, 2, 3]; Ying Zhu[1]; Cong Wang[1]; Dmytro Puchkov[2]; Martin Lehmann[2]; Fan Liu[1, 3]; *[1]Department of Structural Biology, Leibniz Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; [2]Core Facility Cellular Imaging, Leibniz Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany; [3]Charité – Universitätsmedizin Berlin, Berlin, Germany*

WP 698 **An integrated nascent proteomics approach to systematically investigate how translation initiation factors shape the cancer proteome**; Toman Borteçen[1]; Robert Wolfgang Kalis[2]; Johannes Zuber[2]; Jeroen Krijgsveld[1]; Torsten Müller[1]; *[1]German Cancer Resaerch Center (DKFZ), Heidelberg, Germany; [2]Institute 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 Nart[1]; Fatih Aygenli[2]; Tanja Bange[2]; Maria Robles[2]; Jürgen Cox[1]; *[1]Max Planck Institute of Biochemistry, Planegg, Germany; [2]Institute 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 Schmidt[1]; Abigail Mackey[4, 5]; Michael Kjaer[4, 5]; Marcus Krüger[1, 2]; *[1]CECAD research center, Cologne, Germany; [2]Institute for genetics, Cologne University, Cologne, Germany; [3]Center for Molecular Medicine Cologne, Cologne, Germany; [4]ISMC, Department of Orthopedic Surgery, Copenhagen University Hospital - Bispebjerg and Frederiksberg, Copenhagen, Denmark; [5]Department of Clinical Medicine, Faculty of Healthy 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-Mitzner[1]; Kevin Xu[1]; Jin-Hong Du[2]; Bert Klei[3]; Bernie Devlin[3]; Matthew L MacDonald[1, 3]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Carnegie Mellon University, Pittsburgh, PA; [3]University of Pittsburgh Medical Center, Pittsburgh, PA*

WP 702 **MaxQuantAtlas creates large-scale, accurate cellular protein concentration maps from heterogeneous proteomics data**; Daniela Ferretti[1]; Yatao Shi[2]; Pavel Sinitcyn[3]; Shivani Tiwary[3]; Chris Browne[2]; Scott Rusin[2]; Eric Kuhn[2]; Susanne Breitkopf[2]; Sarah Martinez[2]; Dirk Walther[2]; Juergen Cox[1]; Kirti Sharma[2]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Kymera Therapeutics, Watertown, MA; [3]Max 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 Stephens[3]; Richard J Giannone[1]; Evert K Holwerda[3]; Robert L Hettich[1, 2]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Tennessee, Knoxville, TN; [3]Dartmouth 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 Hamerly[1]; Tao Wang[1]; Chris Kwiatkowski[1]; Karina Edwards[1]; Heidi Van Every[1]; Evan Rosa-Roseberry[1]; Francesca Zappacosta[1]; Joseph Kozole[1]; Roland Annan[1]; *[1]GlaxoSmithKline, Collegeville, PA*

WP 705 **USP7 regulates the ncPRC1 Polycomb axis to stimulate genomic H2AK119ub1 deposition uncoupled from H3K27me3**; Jeroen AA Demmers[1]; Ayestha Sijm[1]; Yaser Atlasi[2]; Jan A Van Der Knaap[1]; Joyce Wolf - Van Der Meer[1]; Gillian E Chalkley[1]; Karel Bezstarosti[1]; Dick HW Dekkers[1]; Wouter AS Doff[1]; Zeliha Ozgur[1]; Wilfred FJ Van Ijcken[1]; Peter CP Verrijzer[1]; *[1]Erasmus Medical Center Rotterdam, Rotterdam, Netherlands; [2]Queen's University Belfast, Belfast, United Kingdom*

WP 706 **Proteomic and Transcriptomic analysis of caste transition and aging in the ponerine ant, Harpegnathos saltator**; Maxxum Fioriti[1]; Karl Glastad[2]; Michael Gilbert[1]; Matan Sorek[2]; Tierney Ganon[2]; Shelley Berger[2]; *[1]Department of Biochemistry and Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; [2]Department 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 Lee[1]; Haorong Li[1]; Cha Yang[2]; Jiawei Ni[1]; Wan Nur Atiqah Mazli[1]; Fenghua Hu[2]; Ling Hao[1]; *[1]Department of Chemistry, George Washington University, Washington, DC; [2]Weill 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 Khanijou[1]; Yan Ting Hee[2]; Chew Wee[1]; Kumar Selvarajoo[2, 3, 4]; *[1]Singapore Institute of Food and Biotechnology Innovation, Singapore, Singapore; [2]Bioinformatics Institute (BII), Agency for Science, Technology and Research (A*STAR), Biopolis, Singapore,*

Singapore; [3]Synthetic Biology Translational Research Program & SynCTI, Yong Loo Lin School of Medicine, National University of Singapore (NUS), Kent Ridge, Singapore, Singapore; [4]School 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 Emdal[2]; Anna-Kathrine Pedersen[2]; Rita Slaaby[1]; Peter Kresten Nielsen[1]; Jesper Velgaard Olsen[2]; *[1]Novo Nordisk A/S, Måløv, Denmark; [2]Novo 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 Dong[1]; Qing Yu[1]; Steven R. Shuken[1]; Edward L Huttlin[1]; Steven P Gygi[1]; Joao A Paulo[1]; *[1]Harvard 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 Li[1]; Kaitlyn E. Stepler[1]; Leena R. Pade[1]; Camille Lombard-Banek[1]; Peter Nemes[1]; *[1]University of Maryland College Park, College Park, MD*

WP 712 **Method Development for Epitope Mapping of Membrane Proteins Embedded in Virus-Like Particles**; Esther Wolf[1]; Lauri Peil[2]; Joan Teyra[2]; Mart Ustav Jr. [2]; Derek Wilson[1]; *[1]York University, North York, ON; [2]Icosagen, Ossu, Estonia*

WP 713 **Elucidation of the distinct RNA-protein interactomes of SARS CoV-2 genomic and subgenomic RNAs**; Isabella T Whitworth[1]; Rachel Knoener[1]; Maritza Puray-Chavez[2]; Peter Halfmann[1]; M'bark Baddouh[1]; Sofia Romero[1]; Mark Scalf[1]; Yoshihiro Kawaoka[1]; Sebla Kutluay[2]; Lloyd M Smith[1]; Nathan M Sherer[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Washington University in St. Louis, St Louis, MO*

WP 714 **LC-UV-MS Analysis of Intact Adeno-Associated Virus (AAV) Vector Capsid Proteins**; Amber D Henry[1]; Pei Liu[1]; Kevin Ray[1]; *[1]Sigma Aldrich, St. Louis, MO*

WP 715 **Stability Characterization of Multiple Serotypes of Adeno-Associated Virus Using Charge Detection Mass Spectrometry**; Rachel Koerber[1]; Susan Abbatiello[1]; Andy Jarrell[1]; *[1]Waters 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 Kiyonami[1]; Kristina Srzentic[2]; Kenneth Thompson[3]; Chao Yan Liu[3]; Min Du[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific,, CH-, Switzerland; [3]Thermo Fisher Scientific, Frederick, Maryland; [4]Thermo 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 Jeudy[3]; Adrien Reynaud[4]; Bogdan Vysotskyi[4]; Yohann Couté[2]; Julia Novion-Ducassous[2]; Jean-Michel Claverie[3]; Sébastien Hentz[4]; Chantal Abergel[3]; Christophe Masselon[2]; *[1]Department of Chemistry, National Cheng Kung University, Tainan, Taiwan; [2]UA13, Inserm/CEA/UGA IRIG, Biosciences et bio-ingénierie pour la santé, Grenoble, France; [3]CNRS - UMR 7256 – IGS, IMM-FR 3479, IM2B, IOM, Marseille, France; [4]Université 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 Deng[1]; Jyotsna Kumar[1]; Mikaila French[1]; Daniele Fabris[1]; *[1]UConn 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 Guazzotti[1]; Roxana Eggleston-Rangel[2]; Mastooreh Chamanian[2]; Lorne Nelson[2]; *[1]Phenomenex, Alcobendas, Madrid, Spain; [2]Phenomenex, Torrance, CA*

WP 720 **Peptide mapping and post-translational modifications of AAV5 produced in HEK293**; Geoffrey Rule[1]; Agnieszka Lass-Napiorkowska[2]; Pei Liu[2]; Kevin Ray[2]; Cory Muraco[3]; *[1]Millipore Sigma, Bellefonte, PA; [2]MilliporeSigma, St. Louis, MO; [3]MilliporeSigma, Bellefonte, PA*

WP 721 **Detailed Characterization of Adeno-Associated Virus Capsid Proteins by Combining Peptide Mapping and Protein Fingerprinting by Intact Mass**; Kevin Ray[1]; Pei Liu[1]; *[1]MilliporeSigma, St. Louis, MO*

WP 722 **Arboviral-induced alterations of the mosquito lipidome**; Paul S. Soma[1]; Oshani Ratnayake[1]; Irma Sanchez-Vargas[1]; Nunya Chotiwan[1, 2]; Barbara Graham[1]; Samantha Pinto[1]; Amber Hopf-Jannasch[3]; Rushika Perera[1]; *[1]Center for Metabolism of Infectious Diseases, Center for Vector-borne Infectious Diseases, Colorado State University, Fort Collins, CO; [2]Chakri Naruebodindra Medical Institute, Faculty of Medicine Ramathibodi Hospital, Thailand; [3]Bindley 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 Roudini[3]; Louis Dartiguelongue[2]; Bastien Pellegrin[4]; Sebastien Artous[4]; Andreas Winkler[3]; Christophe Masselon[2]; *[1]University of Grenoble Alpes (UGA), Grenoble, France; [2]CEA, IRIG, Grenoble, France; [3]Leibniz Institute for Solid State and Materials Research, IFW Dresden, Dresden, Germany; [4]CEA, 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 Fortin[2]; Sébastien Hentz[3]; Christophe Masselon[2]; *[1]University of Grenoble Alpes (UGA), Grenoble, France; [2]CEA, IRIG, Grenoble, France; [3]CEA, 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 Sakallioglu[1]; Anjali Alving[1]; *[1]Bruker Scientific, LLC, Billerica, MA*

WP 726 **Development of an LC-MS/MS Based Multi-Attribute Characterization Assay for a Live Virus Vaccine**; David Foreman[1]; Alyssa Q Stiving[1]; Xuanwen Li[1]; Hillary A. Schuessler[1]; *[1]Merck, West Point, PA*

WP 727 **Mass Spectrometry-based Determination of Tailed Phage Virion Protein Copy Number**; Gialinh Vu[1]; Sophia Unwin[1]; Sammy Pardo[2]; Dana Molleur[2]; Susan Ludwigsen[3]; Susan T. Weintraub[2]; Julie A. Thomas[1]; *[1]Rochester Institute of Technology, Rochester, NY; [2]Univ. of Texas HSC, San Antonio, TX; [3]Proteome Software, Portland, OR*

WP 728 **HIV-1 Virion Proteoform Analysis Reveals Conserved and Novel Post-Translation Modifications Modulating Viral Function**; Claire E Boos[1]; James W Bruce[1]; Mark Scalf[1]; Rachel M Miller[1]; Nathan M Sherer[1]; Lloyd M Smith[1]; *[1]University 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. Kafader[1]; John P. McGee[1]; Pei Su[1]; Michael A. R. Hollas[1]; Ryan T. Fellers[1]; Kenneth R Durbin[1]; Philip D. Compton[2]; Neil L. Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Integrated Protein Technologies Inc., Carlsbad, CA*

WP 730 **In-depth Characterization of Adeno-Associated Viruses using Microchip Capillary Electrophoresis Coupled with Mass Spectrometry**; Josh Smith[1]; Sara Carillo[1]; Adi M Kulkarni[2]; Erin Redman[2]; Kate Yu[2]; Jonathan Bones[1, 3]; *[1]National Institute of Bioprocessing Research and Training, Dublin, Ireland; [2]908 Devices, Inc., Boston, MA; [3]School 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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Elemental Analysis...053-054
Energy: Petroleum, Biofuels, and Algae 055-064
Environmental: General III......................................065-089
Environmental: Pharmaceuticals and Pesticides 090-101
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Single Cell MS II 689-713
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 Murdock[1]; Sharon Huws[1]; Simon Cameron[1]; [1]*Queen'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 Palaty[3]; Jason L. Robinson[4]; Christopher G. Gill[1, 2, 5, 6, 7]; [1]*Appl. Env. Res. Labs. (AERL), Nanaimo, BC;* [2]*University of Victoria, Victoria, BC;* [3]*Fraser Health, New Wesminster, BC;* [4]*Health PEI, Charlottetown, PEI;* [5]*Vancouver Island University, Nanaimo, BC;* [6]*Simon Fraser University, Burnaby, BC;* [7]*University 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 Schäffer[2]; Csaba Hajdu[2]; Attila Egri[2]; Fanni Csiza[3]; Bálint András Deák[3]; Benedek Gyöngyösi[3]; Gitta Schlosser[1]; Julia Balog[2]; [1]*Eötvös Loránd University, Budapest, Hungary;* [2]*Waters Research Center, Budapest, Hungary;* [3]*Department 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 Carmany[1]; Nicholas Manicke[2]; Elizabeth Dhummakupt[3]; [1]*Excet, Gunpowder, MD;* [2]*IUPUI, Indianapolis, IN;* [3]*U.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 Perna[1]; Briza Marie Dedicatoria[2]; Ngee Sing Chong[2]; Mengliang Zhang[2]; [1]*Middle Tennessee State University, Murfreesboro, TN;* [2]*Middle Tennesse State University, Murfreesboro, TN*

ThP 006 **Ambient Ionization-Based Screening Protocols for High Priority N-Nitrosamines in Pharmaceutical, Forensic, and Environmental Samples**; Ebenezer H. Bondzie[1]; Trevor J. McDaniel[1]; Patrick W. Fedick[2]; Christopher C. Mulligan[3]; [1]*Illinois state university, Normal, IL;* [2]*Naval Air Warfare Center, Weapons Division, China Lake, CA;* [3]*Illinois 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. Sacks[1]; [1]*Cornell University, Ithaca, NY;* [2]*Bruker 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-Santiago[1]; Rafael Lucena[1]; Soledad Cárdenas[1]; [1]*University of Córdoba, Cordoba, Spain*

ThP 009 **Accelerated Aza-Michael Addition and SuFEx Reaction in Microdroplets**; Jyotirmoy Ghosh[1]; Joshua Mendoza[2]; R. Graham Cooks[2]; [1]*Purdue University, West Lafayette, IN;* [2]*Purdue 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 Schramm[2]; Frédéric Progent[1]; Frédéric Aubriet[2]; [1]*CEA, DAM, DIF, F-91297 Arpajon, France;* [2]*Laboratoire 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 Areces[1]; Daniel Foest[2]; Sebastian Brandt[2]; Juan F. García-Reyes[1]; Joachim Franzke[2]; [1]*University of Jaén, Jaén, Spain;*

[2]Leibniz 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 Oxyphenbutazone in Equine Serum**; David Borts[1]; Laura Burns[1]; Dwayne Schrunk[1]; Tom Kane[2]; Ryan Micklitsch[2]; Shane Stevens[2]; *[1]Iowa State University Veterinary Diagnostic Laboratory, Ames, IA; [2]Restek Corporation, Bellefonte, PA*

ThP 013 **Towards mass spectrometry guided skin cancer surgery**; Lauritz Falkow Brorsen[1, 2, 3]; Fernanda Endringer Pinto[2]; Martin Glud[1]; Stine Regin Wiegell[1]; James McKenzie[3]; Uwe Paasch[4]; Merete Hædersdal[1]; Zoltan Takats[3]; Christian Janfelt[2]; Catharina Margrethe Lerche[1]; *[1]Bispebjerg Hospital, Copenhagen, Denmark; [2]University of Copenhagen, Copenhagen, Denmark; [3]Imperial College, London, London, United Kingdom; [4]University 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. Kalenak[1]; Terry L Bates[1]; Gavin L. Sacks[1]; *[1]Cornell 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 Zhang[1]; Michael Loomer[1]; Ejoke Akatugba[1]; Gerardo Gamez[1]; *[1]Texas Tech University, Lubbock, TX*

ThP 016 **Direct analysis and classification of different olive oils by paper spray mass spectrometry**; Ines R Talarico[1]; Lucia Bartella[1]; Priscilla Rocio Bautista[2]; Antonio Molina Díaz[3]; Leonardo Di Donna[1]; Juan F Garcia-Reyes[3]; *[1]University of Calabria, Rende, Italy; [2]Universidad de Jaen, Jaén, Spain; [3]UNIVERSITY OF JAEN, Jaen, Spain*

ThP 017 **A Tool Allowing Rapid Acquisition and Extraction for Processing of DESI Screening Application Data**; Mark Towers[1]; Lisa Reid[1]; Richard Chapman[2]; Joanne B Ballantyne[1]; Royston Goodacre[3]; Ian D Wilson[3]; Paul Richardson[3]; Richard Daw[4]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, Milford, MA; [3]University of Liverpool, Liverpool, United Kingdom; [4]Waters 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. Proctor[1]; Youwen You[1]; Jaclyn R. Missanelli[1]; Cynthia Otto[2]; Mary A. Robinson[1]; *[1]University of Pennsylvania, West Chester, PA; [2]University of Pennsylvania, Philadelphia, PA*

ThP 020 **Automating analyses of confiscated samples for identification of illicit drugs**; Fuyu Guan[1]; Savannah Fay[2]; Matthew A. Adreance[1]; Leif McGoldrick[1]; Rachel M. Proctor[1]; Jaclyn R. Missanelli[1]; Youwen You[1]; Mary A. Robinson[1]; *[1]University of Pennsylvania, West Chester, PA; [2]Katherine 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. Missanelli[1]; Youwen You[1]; Rachel M. Proctor[1]; Joanne Haughan[1]; Mary A. Robinson[1]; *[1]University 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]; *[1]Department of Clinical Studies, School of Veterinary Medicine, University of Pennsylvania, New Bolton Center Campus, Kennett Square, PA; [2]Pennsylvania 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 Soboń[1, 2]; Rafał Szewczyk[1, 2]; Anna Lenartowicz[1]; Julia Mironenka[1]; Katarzyna Krupczyńska-Stopa[1, 2]; Maciej Stopa[1, 2]; Andrzej Kwaśnica[3]; *[1]LabExperts sp. z o. o., Gdańsk, Poland; [2]Bioanalytic sp. z o. o., Gdańsk, Poland; [3]Lab4Tox 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 Kang[1]; Junghyun Son[1]; Eugene C. Yi[2]; Hophil Min[1]; *[1]Korea institute of science and technology, Seoul, South Korea; [2]Seoul National University, Seoul, South Korea; [3]Korea university, Seoul, South Korea*

ThP 025 **Using Water Adduction to Differentiate Cannabinoid Isomers in a Quadrupole Ion Trap Mass Spectrometer**; Dinuri S. Fernando[1]; Cameron D. Worthington[1]; Gary L. Glish[1]; *[1]University 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 Seale[3]; Brett Larson[3]; Anne-Claude Gingras[1, 3]; Hannes L Röst[1, 2]; *[1]Department of Molecular Genetics, University of Toronto, Toronto, ON; [2]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto Toronto, ON, Canada, Toronto, ON; [3]Lunenfeld-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 Morrice[1]; Ihor Batruch[2]; Patrick Pribil[2]; *[1]SCIEX, Macclesfield, United Kingdom; [2]SCIEX, Concord, ON*

ThP 028 **Integrating DIA-NN software analysis of data-independent acquisition data into a cloud processing pipeline**; Melanie Juba[1]; Nick Morrice[2]; Alexandra Antonoplis[3]; Christie Hunter[3]; Patrick Pribil[4]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Alderley Park, United Kingdom; [3]SCIEX, Redwood city, CA; [4]SCIEX, 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 Rijal[1]; Christine Schaeffer[1]; Christine Carapito[1]; *[1]Laboratoire 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 Alexeev[1]; Juergen Cox[1]; *[1]Max 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 Pérez[3]; Qian Ba[1]; Alison M. Taylor[3]; Yansheng Liu[1, 2]; *[1]Yale University, New Haven, CT; [2]Yale Cancer Biology Institute, West Haven, CT; [3]Columbia University, New York, NY*

ThP 032 **DIA Phosphoproteomics: Comparative Evaluation of Dynamic Range and Quantitative Accuracy across Multiple MS Platforms**; Tanmayi D Vashist[1]; Alvaro Sebastian Vaca[1, 2]; Claudia Ctortecka[1]; Khoi Pham Munchic[1]; Hasmik Keshishian[1]; D. R. Mani[1]; Shankha Satpathy[1]; Steven A Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Bruker Daltonics, Billerica, MA*

ThP 033 **Improved library free dia-PASEF based quantitative proteomics using Spectronaut**; Tejas Gandhi[1]; Oliver M Bernhardt[1]; Véronique Laforte[1]; Damiano Robbiani[1]; Anna Susmelj[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

ThP 034 **Accelerated mass spectrometry imaging via MS/MS spectrum deconvolution of inter-pixel compositional variations of metabolites**; Dan Li[1]; Zheng Ouyang[1]; Xiaoxiao Ma[1]; *[1]State Key Laboratory of Precision*

Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University,, Beijing, China

ThP 035 **From data-independent acquisition (DIA) to targeted MS/MS: Automatic reinjection for additional confirmation in suspect screening**; Christian Klein[1]; James S Pyke[1]; Emma E Rennie[1]; Cate Simmermaker[1]; Karen E Yannell[1]; Madhusudan Sharma[1]; Li Sun[1]; Kai Chen[1]; *[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 Liu[1]; Tess Puopolo[1]; Huifang Li[1]; Ang Cai[1]; Hang Ma[1]; Navindra P Seeram[1]; *[1]University of Rhode Island, Kingston, RI*

ThP 037 **DirectDIA+ improves library free quantification for plasma proteomics**; Damiano Robbiani[1]; Tejas Gandhi[1]; Lukas Reiter[2]; Oliver M Bernhardt[2]; Roland Bruderer[1]; *[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 Wang[1]; Gang Xin[1, 4]; Amanda B. Hummon[1, 3]; Brian C Searle[2]; *[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 Franco[1]; Cecily R Wood[1]; Alison Porter[1]; Scott M Peterman[2]; Scott D Stanley[1]; *[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 Qiu[3]; Vladimir Ignatchenko[2]; Julius O Nyalwidhe[4, 5]; O. John Semmes[4]; 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. Zolg[1]; Tobias Schmidt[1]; Siegfried Gessulat[1]; Florian Seefried[1]; Michael Graber[1]; Samia Ben Fredj[1]; Patroklos Samaras[1]; Markus Schneider[1]; Layla Eljagh[1]; Vishal Sukumar[1]; Pedro Navarro[2]; Kai Fritzemeier[2]; Yovany Cordero Hernandez[2]; Frank Berg[2]; Carmen Paschke[2]; David Horn[3]; Bernard Delanghe[2]; Christoph Henrich[2]; Mathias Wilhelm[4]; Martin Heinrich Frejno[1]; *[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 Blanc[1]; Eva Duchoslav[1]; Lyle Burton[1]; Stephen Tate[2]; Bradley Schneider[2]; *[1]SCIEX, Concord, On, ON; [2]SCIEX, Concord, ON*

ThP 043 **Investigation of the human lysosomal proteome by targeted proteomics**; Stephanie Kaspar-Schoenefeld[1]; Dhriti Arora[2]; Andreas Schmidt[1]; Dominic Winter[2]; *[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 King[1]; Shweta S Dipali[2]; Francesca E Duncan[1, 2]; Birgit Schilling[1]; *[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 Pichler[1]; Manuel Matzinger[1]; Goran Mitulovic[2]; Karl Mechtler[1]; *[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 Bu[1]; Junhan Wu[2]; Nan Zhang[1]; Yuyu Li[1]; Wenpeng Zhang[2]; Zheng Ouyang[2]; *[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 Mongane[1]; Luke A Squires[1]; Alyssa A Nitz[1]; Samuel H Payne[1]; *[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 Mathews[1]; Claudia M Boot[1]; *[1]Colorado State University, Fort Collins, CO*

ThP 050 **Benchtop MALDI MSI: Mass Spectrometry Imaging on a Budget**; Kendra G. Selby[1]; Emily M Hubecky[1]; Gabriel A. Bressendorff[1]; Ashley R Chirchirillo[1]; Summy Shrestha[1]; Lynne Ling[2]; Donald Caspary[2]; Kevin R Tucker[1]; *[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; *Louisiana State University, Baton Rouge, LA*

ThP 052 **Unlocking the Power of Mass Spectrometry in Biomanufacturing: A Microlearning Approach**; M. Cyndell Gracieux-Singleton[1]; Jason Whitley[1]; Brian Herring[1]; Marie Vestergaard[2]; Scott Latus[1]; *[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 Bian[1]; Aimei Zou[1]; Patrick Simmons[2]; *[1]Agilent Technologies, Singapore, Singapore; [2]Agilent Technologies, Santa Clara, CA*

ThP 054 **Mpx/hr LA-ICP-TOFMS mapping and data evaluation**; Martin Rittner[1]; Steffen Bräkling[1]; David Douglas[2]; Bence Paul[3]; *[1]TOFWERK, Gwatt (Thun), Switzerland; [2]Elemental Scientific Lasers, Huntington, United Kingdom; [3]Elemental Scientific Inc, Melbourne, Australia*

ThP 055 **Effects of Aromaticity on Petroleum Acid Fragmentation**; Esther Mbuna[1]; Nathan Gard[1]; Andrew Adam[1]; Benjamin Bythell[1]; [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 Dreschmann[1]; Wolfgang Schrader[1]; [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 Denson[2]; Raiza Manrique Waldo[3]; Anthony Dufour[4]; Vincent Carre[5]; Frederic Aubriet[5]; Manuel Garcia-Perez[2]; [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 ofNaphthenic acids from Oil**; Sol Sauna Nety[1]; Simiso Dube[1]; Mathew M Nindi[2]; [1]*University of South Africa, Johannesburg, South Africa;* [2]*UNISA, Florida Park, Roodepoort, South Africa*

ThP 060 **Derivatized Carbazoles Dissociation Chemistry**; Dylan Carter[1]; Jaya Paudel[1]; Benjamin Bythell[1]; [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 Vetere[1]; Wolfgang Schrader[1]; [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 Choe[1]; Mike Jindra[2]; Susan Hubbard[2]; Blake Mirman[1]; Brian F Pfleger[2]; Jonathan V. Sweedler[1]; [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 Paudel[1]; Lauren Davis[1]; Dylan Carter[1]; Benjamin Bythell[1]; [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 Kousar[1]; Timo Kekäläinen[1]; Matthias Witt[2]; Janne Janis[1]; [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 Smolinski[1]; Meghan Oates[2]; Amith Maroli[2]; Arjun Venkatesan[2, 3]; Carrie A McDonough[1]; [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 Camdzic[1]; Rebecca A. Dickman[1]; Abigail S. Joyce[2]; Joshua S. Wallace[1]; P. Lee Ferguson[2]; Diana S. Aga[1]; [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-Al Hassan[1]; Praneeth Ivan Joel Fnu[1]; Yongling Ai[1]; Francis J. Osonga[1]; Omowunmi A. Sadik[1]; Mengyan Li[1]; Hao Chen[1]; [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 Napolitano[1]; Zijie Beryl Xia[2]; Alexander Schrum[1]; Ronald Benson[1]; [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 Park[1]; Seungwoo Son[1]; Yonghyeon Yim[2]; 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. Boatman[1]; Kylie D. Rock[2]; Scott M. Belcher[2]; Erin S Baker[1]; [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 Alam[1]; Dede Heri Yuli Yanto[2]; 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 Dowd[1]; Kari Organtini[1]; Marian Twohig[1]; Jean Carlan[2]; 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 Shrestha[1]; Ethan Hain[1]; Kathleen Luo[1]; Christopher Gilles[1]; Evelyn Wang[1]; Xiaomeng Xia[1]; Robert English[1]; Tiffany Liden[1]; [1]*Shimadzu Scientific Instruments, Columbia, MD*

ThP 074 **Extremely sensitive, real-time detection of PFAS in the gas phase**; Joel R. Kimmel[1]; Abigail Koss[1]; Carla Frege[2]; [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 Luo[1]; Emily Parry[1]; Matthew Giardina[1]; Linfeng Wu[1]; Patrick Batoon[1]; Tarun Anumol[1]; [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 Kiridena[1]; Manjula M Kandage[1]; Norman Peiffer[2]; Michal Marszewski[1]; Dragan Isailovic[1]; [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 Nguyen[1]; O. David Sparkman[1]; Liang Xue[1]; Harry Allen[2]; Terry Ramus[3]; [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

Schrader[1]; Ruoji Luo[1]; Ilker Satilmis[1]; *[1]Max-P'lanck Institut für Kohlenforschung, Mülheim, Germany*

ThP 079 **New Directions in wastewater-based epidemiology. Identification of small and large biomolecules as biomarkers of public health and industrial activities**; Ruben Gil Solsona[1]; Jessica Subirats[1]; Montserrat Carrascal[2]; Pablo Gago Ferrero[1]; Antoni Ginebreda[1]; Damia Barcelo[1, 3]; *[1]IDAEA-CSIC, Barcelona, Spain; [2]Info Institut d'Investigacions Biomèdiques August Pi i Sunyer, Barcelona, Spain; [3]Catalan 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 Liu[1]; Michael Shields[1]; Sangeetha Puthigai[1]; Xiaolei Xu[1]; Shari Yvon-Lewis[1]; *[1]Texas 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 Zhang[1]; Courtney C. Carignan[2]; Taylor Hoxie[1]; Heather M Stapleton[1]; *[1]Duke University, Durham, NC; [2]Michigan 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 Weed[1]; Jeffrey Enders[1]; Grace Campbell[1]; Katlyn May[1]; *[1]North 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 Thenuwara[1]; Nicholas J Peraino[2]; Judy A Westrick[2]; Dragan Isailovic[1]; *[1]University of Toledo, Toledo, OH; [2]Wayne State University, Detroit , MI*

ThP 084 **Non-Targeted Analysis of Emerging Per- and Polyfluoroalkyl Substances (PFAS) in Rainwater**; Yubin Kim[1]; Kyndal A. Pike[1, 2]; Donald Conley[1]; Jameson Sprankle[1]; Rebekah Gray[1]; Christopher Alaimo[3]; Thomas Young[3]; Jennifer Faust[1]; Paul L Edmiston[1]; *[1]College of Wooster, Wooster, OH; [2]University of Wisconsin-Madison, Madison, WI; [3]University of California, Davis, Davis, CA*

ThP 085 **Untargeted Exposure Analysis of Lake Okeechobee Using SPE-UHPLC-HRMS**; Jae Hwan Lee[1]; Ellen Titus[2]; Krista McCoy[2]; Timothy J. Garrett[1]; *[1]University of Florida, Gainesville, FL; [2]Florida 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 Kudzin[1]; James N Dodds[1]; Hannah Starnes[2]; Zach Mclean[2]; Scott M. Belcher[2]; Erin S Baker[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]North Carolina State University, Raleigh, NC*

ThP 087 **GC-MS method with reduced solvent consumption for PBDE quantification in revalorized polymers**; Marc-Antoine Vaudreuil[1]; Richard Silverwood[2]; Alexandra Furtos-Matei[1]; *[1]Université de Montréal, Montreal, QC; [2]Lavergne Inc., Montreal, QC*

ThP 088 **Direct filter desorption of environmentally relevant chemicals using multi-scheme chemical ionization (MION) mass spectrometry**; Joona Mikkilä[1]; Fariba Partovi[1, 2]; Jyri Mikkilä[1]; Tuija Jokinen[3]; Neha Deot[3]; Mikko J Sipilä[4]; Aleksei Shcherbinin[1]; Matti P Rissanen[2]; Hj Jost[1]; *[1]Karsa Ltd, Helsinki, Finland; [2]Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; [3]Climate and Atmosphere Research Center (CARE-C), The Cyprus Institute, Nikosia, Cyprus; [4]Institute 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 Rosales[1]; Krysten L Sheedy[1]; Karl V Wasslen[1]; Jeffrey M Manthorpe[1]; Jeffrey C Smith[1]; *[1]Carleton University, Ottawa, ON*

ThP 090 **Streamlining HRMS data acquisition and interpretation for wastewater impact on water quality**; Michael Thurman[1]; Imma Ferrer[1]; James S Pyke[2]; *[1]University of Colorado, Boulder, CO; [2]Agilent 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**; Xiaoou Wei[1, 2, 3]; Yujie Ben[3]; Chunmiao Zheng[3, 4]; Zongwei Cai[1, 2]; *[1]State Key Laboratory of Environmental and Biological Analysis, Hong Kong Baptist University, Hong Kong, China; [2]Department of Chemistry, Hong Kong Baptist University, Hong Kong, China; [3]State 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; [4]EIT 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 Giraud[1]; Yves Leblanc[2]; Mircea Guna[2]; Gérard Hopfgartner[1]; *[1]LSMS, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; [2]SCIEX, 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 Kim[1]; Sung-Gil Choi[1]; Young Sang Kwon[1]; Deuk-Yeong Lee[2]; Jong-Su Seo[1]; Jong-Hwan Kim[1]; *[1]Environmental Safety Assessment Center, Gyeongnam Branch Institute, Korea Institute of Toxicology, Jinju, South Korea; [2]Residue 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 Pudenzi[1]; Luis Otavio Junqueira[1]; *[1]Shimadzu do Brasil LTDA, Barueri, Brazil*

ThP 096 **Determination of multiresidue pesticides in Arabian Dates using LC and GC Triple Quadrupole Mass Spectrometry**; Tuna Oncu[1]; Orhan Papak[1]; *[1]Shimadzu 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 Copling[1]; Jacob Smith[2]; Katherine Maloof[2]; Jacob Pierson[2]; Hannah Konschak[2]; Leslie Kupferle[2]; Adam Sullivan[2]; Megan Davis[2]; Chloe Pancake[2]; Samuel Bickford[2]; Robert Dixon[2]; Kevin R Tucker[2]; *[1]Southern Illinois University of Edwardsville, White/Caucasian, IL; [2]Southern 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]; Joona Mikkilä[2]; Jussi Kontro[2]; Jyri Mikkilä[2]; Nasib Naseri[2]; Aleksei Shcherbinin[2]; Paxton Juuti[2]; Suvi Ojanperä[3]; Matti Rissanen[4, 5]; *[1]Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; [2]Karsa Ltd., Helsinki, Finland; [3]Finnish Customs, Helsinki, Finland; [4]Aerosol Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, Tampere, Finland; [5]Department 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 Damale[1]; Jessin Mathai[1]; Kumar

Raju[1]; Rajendra Makhamale[1]; Atul Narkar[1]; *[1]Shimadzu Middle East & Africa FZE, Dubai, United Arab Emirates*

ThP 100 **Rapid low-cost testing of urine for unknown pesticide variants**; Alexey Melnik[1, 2]; Olusola Onawoga[2]; David Chick[2]; Silverio Iacono[2, 3]; Alexander Aksenov[2, 4]; *[1]University of Connecticut, Storrs, CT; [2]Arome Science Inc., Farmington, CT; [3]TomTec, Hamden, CT; [4]University of Connecticutt, Storrs, CT*

ThP 101 **Impact of Using 1.5 mm Column ID and Various Stationary Phases on LC/MS Pesticide Screening Analysis**; Stephanie Schuster[1]; Peter Pellegrinelli[1]; Conner W. McHale[1]; Benjamin Libert[1]; Taylor Harmon[1]; *[1]Advanced Materials Technology, Inc., Wilmington, DE*

ThP 102 **FluoroMatch 3.0 – Automated PFAS Non-Targeted Analysis and Visualizations Applied to Mammalian Biofluids**; Michael Kummer[1]; Nandarani Abril[1]; Emily Parri[2]; Sheng Liu[3]; Carrie A McDonough[4]; David Dukes[5]; David Godri[6]; Elizabeth Z. Lin[3]; Emma E Rennie[2]; Jeremy Koelmel[3]; Krystal JG Pollitt[3]; *[1]Innovative Omics, Sarasota, FL; [2]Agilent Technologies, Santa Clara, CA; [3]Yale University, New Haven, CT; [4]Carnegie Mellon University, Pittsburgh, PA; [5]Stony Brook University, Stony Brook, NY; [6]3rd 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-Thurnherr[3]; Benedikt Warth[1, 2]; *[1]University of Vienna, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Währinger Straβe 38, 1090, Vienna, Austria; [2]Exposome Austria, Research Infrastructure and National EIRENE Hub, Vienna, Austria; [3]Empa, 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 McEachran[1]; Tristan Chutka[1]; Alex Chao[2]; Gregory Janesch[3]; Elin Ulrich[2]; Jon Sobus[2]; Antony Williams[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Chemical Characterization and Exposure Division, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, NC; [3]ORAU 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 Möller[1]; Alexandra Keidel[2]; Jazmine Virzi[1]; Laura Deloso[2]; Yuan-Jhe Chang[3]; Mu-Rong Chao[3, 4]; Chiung-Wen Hu[5]; Marcus S. Cooke[1]; *[1]Oxidative Stress Group, Department of Molecular Biosciences, University of South Florida, Tampa, Florida 33620; [2]Department of Chemistry, University of South Florida, Tampa, Florida 33620; [3]Department of Occupational Safety and Health, Chung Shan Medical University, Taichung, Taiwan; [4]Department of Occupational Medicine, Chung Shan Medical University Hospital, Taichung, Taiwan; [5]Department 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 Chen[1]; Zhengzhi Xie[1]; Maleesha De Silva[1]; Saurin R. Sutaria[1]; Hong Gao[1]; Sanjay Srivastava[1]; Pawel Lorkiewicz[1]; *[1]University of Louisville, Louisville, KY*

ThP 107 **Roles of HNOx and Carboxylic Acids in Thermal Stability of Nitroplasticizers**; Kitmin Chen[1]; Dali Yang[1]; Zheng-hua Li[1]; Oana C. Marina[1]; Alexander S. Edgar[1]; *[1]Los 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 Lai[1]; Yujia Zhao[2]; Douglas I. Walker[3]; Christina M. Lill[4, 5]; Bastiaan R. Bloem[6]; Sirwan K.L. Darweesh[6]; Susan Peters[2]; Roel Vermeulen[2, 7]; Gary W. Miller[1]; *[1]Department of Environmental Health Sciences, Mailman School of Public Health, Columbia University, New York City, NY; [2]Institute for Risk Assessment Sciences, Utrecht University, Utrecht, Netherlands; [3]Department of Environmental Health, Rollins School of Public Health, Emory University, Atlanta, GA; [4]Institute of Epidemiology and Social Medicine, University of Münster, Münster, Germany; [5]School of Public Health, Imperial College London, London, United Kingdom; [6]Radboud University Medical Center; Donders Institute for Brain, Cognition and Behaviour; Department of Neurology; Center of Expertise for Parkinson & Movement Disorders, Nijmegen, Netherlands; [7]University Medical Centre Utrecht, Utrecht, Netherlands*

ThP 109 **Wristband Personal Passive Samplers and Suspect Screening Methods Highlight Gender Disparities in Chemical Exposures**; Nicholas Herkert[1]; Jessica L Levasseur[1]; Kate Hoffman[1]; Gordon Getzinger[2]; P. Lee Ferguson[2]; Anna S Young[3]; Joseph G Allen[3]; Elizabeth Z Lin[4]; Krystal J Godri Pollitt[4]; Heather M Stapleton[1]; *[1]Nicholas School of the Environment, Duke University, Durham, NC; [2]Department of Civil and Environmental Engineering, Duke University, Durham, NC; [3]Department of Environmental Health, Harvard T.H. Chan School of Public Health,, Boston, MA; [4]Department 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 Weldemariam[1]; Tao Ma[2]; Sarah L.J. Michel[1]; Richard N. Dalby[1]; Abraham Schneider[2]; Maureen A. Kane[1]; *[1]Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, Maryland; [2]Department 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 Chovatiya[1]; Ravikumar Jagani[1]; Manish Arora[1]; Syam S. Andra[1]; *[1]Institute 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 Zheng[1]; Lun Zhang[1]; Mathew Johnson[1]; Rupasri Mandal[1]; David S. Wishart[1]; *[1]University of Alberta, Edmonton, AB*

ThP 113 **Mapping the exposome of firefighters through the lens of mass spectrometry**; Xiangping Lin[1]; Xinyue Zhang[1]; Basil Michael[1]; Frank Wong[1]; Mary Prunicki[2]; Kari Christine Nadeau[2]; Michael P. Snyder[1]; *[1]Department of Genetics, Stanford University, Stanford, CA; [2]Sean 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]; *[1]University of Quebec in Montreal, Montreal, QC; [2]EcotoQ network on ecotoxicology research, Quebec, QC; [3]University 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 Xie[1]; Saurin R. Sutaria[1]; Jin Y. Chen[1]; Hong Gao[1]; Daniel J. Conklin[1]; Rachel J. Keith[1]; Sanjay Srivastava[1]; Aruni Bhatnagar[1]; Pawel Lorkiewicz[1]; *[1]University 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 Lee[2]; Christin Duran[2]; John T Kelly[3]; Mitch Rubenstein[3]; *[1]UES, DAYTON, Ohio; [2]AFRL, 711th Human Performance Wing, DAYTON, Ohio; [3]US AIR FORCE, DAYTON, OH*

ThP 117 **Liquid chromatographic retention time prediction models to secure and improve the feature annotation process in high-resolution mass spectrometry**; Julien Parinet[1]; Yassine Makni[2]; Thierno Diallo[2]; Thierry Guérin[1]; *[1]ANSES, Maisons-Alfort, France; [2]ANSES Maisons-Alfort, Maisons-Alfort, France*

ThP 118 **Effect of environmental exposome on early childhood atopic dermatitis**; Su Jung Kim[1]; Mi Jeong Kim[1]; Hyo Yeong Lee[1]; Hyun Ju Yoo[1]; *[1]Asan Medical Center, Seoul, South Korea*

ThP 119 **Quality Control of Electronic-Cigarette Liquids by Helium-Plasma Ionization (HePI) Mass Spectrometry**; Kinan Khanzada[1]; Logan Buddenbaum[1]; Sihang Xu[1]; Athula B. Attygalle[1]; David Douce[2]; Steve Bajic[2]; *[1]Stevens Institute of Technology, Hoboken, NJ; [2]Waters Corporation, Milford, Milford, MA*

ThP 120 **Consumer Product Non-targeted Exposomics for Prospective Human Health**; Jenna Hua[1]; Kristin A Favela[2]; William D Watson[2]; Jake A Janssen[2]; Michael J Harnett[2]; Heath A Spidle[2]; Jarod Grossman[1, 3]; *[1]Million Marker Wellness, Inc., Berkeley, CA; [2]Southwest Research Institute, San Antonio, TX; [3]Agilent Technologies, Santa Clara, CA*

ThP 121 **Comparison of Targeted and Untargeted DNA Adductomics methods on an LC/qToF platform**; Nathan Montgomery[1]; Corey Broeckling[1]; *[1]Colorado 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 Sun[1]; Mengliang Zhang[2]; Nicola Kubzdela[1]; Yaguang Luo[1]; James Harnly[1]; Pei Chen[1]; *[1]USDA-ARS, Beltsivlle, MD; [2]Middle Tennesse State University, Murfreesboro, TN*

ThP 123 **Nitrofuran 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 Liu[2]; Chen-Ting Wu[3]; *[1]Institute of Environmental and Occupational Health Sciences, National Yang Ming Chiao Tung University, Taipei, Taiwan; [2]Department of Safety, Health and Environmental Engineering, National United University, Miaoli, Taiwan; [3]Institute 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 Thompson[1]; Sue D'Antonio[2]; Donna Payne[3]; Hui Zhao[2]; Mike Adams[4]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Wilmington, Delaware; [3]AnalytEval, SMITHVILLE, TX; [4]CWC Labs, Smithville, TX*

ThP 126 **Micro-QuEChERS coupled with UHPLC-MS/MS for Determination of Benzophenones and Parabens from Tea in Taiwan**; Chen-Ting Wu[1]; Yu-Fang Huang[2]; *[1]Institute of Food Safety and Health Risk Assessment, National Yang Ming Chiao Tung University, Taipei, Taiwan; [2]Institute 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 Zhao[1]; Xiaogang Zhang[2]; Zong Yang[3]; Bingjie Liu[3]; Lihai Guo[3]; *[1]SCIEX, Shanghai, China; [2]SCIEX, shanghai, China; [3]SCIEX, Shanghai, China*

ThP 128 **Development of a Multi Analyte Method for the Screening of Dietary Supplement Products**; Christopher R. Beekman[1]; Rahul Pawar[1]; *[1]U.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 Jun[1]; Kyungdo Kim[1]; Zee-Yong Park[1]; Sangsuk Oh[2]; *[1]School of Life Science, Gwangju Institute of Science and Technology, Cheomdangwagiro123, Buk-gu, Gwangju, South Korea; [2]Department 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 Zhang[1]; Philip Johnson[1]; Melanie Downs[1]; *[1]Food 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 Salivo[1]; Tom K. Abban[1]; Matthew E. Openshaw[1]; Reda Hamour[2]; *[1]Shimadzu, Manchester, UK, Manchester, United Kingdom; [2]Shimadzu France, Marne La Vallee, France*

ThP 132 **Tracing the origins of red cabbage moss using a QTOF instrument for rapid nutrient identification**; Qing Liu[1]; Liu qing Zhao[2]; Zong Yang[3]; Bing jie Liu[4]; Li hai Guo[5]; *[1]SCIEX, nanchang, China; [2]SCIEX, Shanghai, China; [3]SCIEX, Shanghai, China; [4]SCIEX, Beijing, China; [5]SCIEX, China, Beijing, China*

ThP 133 **Quantitation of Polysaccharides in food using LC-MS/MS**; Jiani Jiang[1]; Nikita P. Bacalzo, Jr. [1]; Carlito B. Lebrilla[1]; *[1]University of California, Davis, Davis, CA*

ThP 134 **Immunoaffinity Plastic Blade Spray Mass Spectrometry for Rapid Confirmatory Analysis of Food Contaminants1**; Ariadni Geballa-Koukoula[1]; Arjen Gerssen[1]; Marco Blokland[1]; Michel Nielen[1, 2]; *[1]Wageningen Food Safety Research (WFSR) part of Wageningen University & Research, Wageningen, Netherlands; [2]Laboratory 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 Kwon[1]; Hyojin Hwang[1]; Jeongkwon Kim[1]; *[1]Department of Chemistry, Chungnam National University, Daejeon, South Korea*

ThP 136 **High-throughput UHPLC-MS/MS Analyses Optimizing the Flavor of Dairy Products**; Florian Utz[1]; Andrea Spaccasassi[1]; Timo D. Stark[1]; Johanna Kreissl[2]; Caren Tanger[3]; Ulrich Kulozik[3]; Thomas F. Hofmann[1]; Corinna Dawid[1]; *[1]Chair of Food Chemistry and Molecular Sensory Science, Technical University of Munich, Freising, Germany; [2]Leibniz-Institute for Food Systems Biology at the Technical University of Munich, Freising, Germany; [3]Chair 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 Prenni[1]; Jacqueline Chaparro[1]; Corey Broeckling[1]; Nathan Montgomery[1]; Nichole Reisdorph[2]; Richard Reisdorph[2]; Cole Michael[2]; Katrina A Doenges[2]; Arpana Vaniya[3]; Oliver Fiehn[3]; Stacy D Sherrod[4]; Katrina L. Leaptrot[4]; Jody C. May[4]; John A. McLean[4]; Chi-Ming Chien[5]; Tracy Shafizadeh[5]; Steve Watkins[5]; *[1]Colorado State University, Fort Collins, CO; [2]University of Colorado Anschutz, Denver, CO; [3]University of California Davis, Davis, CA; [4]Vanderbilt University, Nashville, TN; [5]Verso Biosciences, San Francisco, CA*

ThP 138 **Rapid Authentication of Red Wine by MALDI-MS Combined with DART-MS**; Xuewei Lin[1]; Hao Wu[2]; Gefei Huang[1]; Qian Wu[1]; Zhongping Yao[1]; *[1]The Hong Kong Polytechnic University, Kowloon, Hong Kong; [2]Xiamen University, Xiamen, China*

ThP 139 **Comprehensive analysis of functional ingredients using LC-MS/MS**; Kazuya Katada[1, 2]; Mami Okamoto[1]; Jun Watanabe[1]; Atsuhiko Toyama[1]; Mari Maeda-Yamamoto[2, 3]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Self Care Food Council, Chiyoda-Ku, Japan; [3]National Agriculture and Food Research Organization, Tsukuba, Japan*

ThP 140 **Retrospective screening of unknown emerging contaminants in tea using LC-HRMS**; Gui-Ru Xie[1]; HONG-JHANG Chen[2]; *[1]Health and Nutrition, SGS Taiwan*

Ltd, New Taipei City, Taiwan; [2]Institute 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 Iida[1]; Kaoru Nakagawa[1]; Manami Kobayashi[2]; *[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. Butler[1]; Erica Bakota[2]; Christine M. Fisher[3]; Brian Ng[3]; Ann M. Knolhoff[3]; *[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 Bowman[1]; Daniel Lukas[1]; Paul M Zelisko[1]; Wendy E Ward[1]; *[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 Sekimoto[1]; Yuto Nishikido[1]; Toshio Hanada[2]; Kazuhisa Uchiyama[3]; Katsuhiro Shiratake[4]; *[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 Tzavellas[1]; Ioannis Martakos[1]; Marilena Dasenaki[1]; Ioannis Skoufos[2]; Athina Tzora[2]; Evagelos Gikas[1]; Kevin Stup[3]; Carsten Baessmann[4]; Nikolaos S. Thomaidis[1]; *[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. Hughey[1]; Amanda R Cicali[1]; Angelina V Lo Presti[1]; Lynn E Marsh[1]; Ashleigh E Outhous[1]; Leighann R Weber[1]; Steve Harper[1]; Samuel A Morton[1]; *[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 Martakos[1]; Ilias Tzavellas[1]; Marilena Dasenaki[1]; Ioannis Skoufos[2]; Athina Tzora[2]; Charalampos Proestos[1]; Brian Teeter[3]; Carsten Baessmann[4]; Nikolaos S. Thomaidis[1]; *[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 $[O=U\equiv CH]^+$, $[U\text{-}H]^+$, and U^+**; Justin Terhorst[1]; Samuel Lenze[2]; Michael Van Stipdonk[2]; *[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 Buenger[1]; Paul M. Mayer[1]; *[1]University of Ottawa, Ottawa, ON*

ThP 150 **Dissociation Chemistry of Substituted Indolines**; Lauren Elizabeth Davis[1]; Esther Mbuna[1]; Benjamin Bythell[1]; *[1]Ohio University, Athens, OH*

ThP 151 **Revisiting the Fragmentation Mechanism of Catechin Isomers**; Kuok-Fai Li[1]; Pai-Chi Syue[1]; Kuo-Lung Ku[1]; *[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 Mismash[1]; Savannah R Porter[1]; Andrew J Arslanian[1, 2]; Bryce J Davis[1]; Tanner Taylor[1]; David V Dearden[1]; *[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 Lantz[1]; Robert Schrader[1]; Mirabel Sun[1]; Joseph Meeuwsen[2]; Jared Shaw[2]; Joseph Beckman[2]; David Russell[1]; *[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 Lieu[1]; Joshua Hinkle[2]; John E.P. Syka[2]; 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 Papanastasiou[1]; Athanasios Smyrnakis[1]; Alexandros Lekkas[1]; Mariangela Kosmopoulou[1]; *[1]Fasmatech, NCSR Demokritos, Athens, Greece*

ThP 156 **Unexpected Gas-Phase Nitrogen-Oxygen Smiles Rearrangement: Collision-induced Dissociation of Deprotonated 2-(N-Methylanilino)ethanol and Morpholinylbenzoic Acid Derivatives**; Yuxue Liang[1]; Yamil Simón-Manso[2]; Pedatsur Neta[2]; Xiaoyu Yang[2]; Yi Liu[1]; Tallat Bukhari[2]; Stephen E. Stein[2]; *[1]National Institute of Standards and Technology, Gaithersburg, MD; [2]National Institute for Standards and Technology, Gaithersburg, MD*

ThP 157 **Exploration of UVPD fragmentation trends of peptides generated by MALDI**; Sean D Dunham[1]; Erin H. Seeley[1]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

ThP 158 **Operation of Simple SID Devices using Two or Three Voltages**; Andrew J Arslanian[1]; Leon (Yu-Fu) Lin[1]; Arpad Somogyi[1]; Vicki H Wysocki[1]; *[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 Gadkari[1]; Rowan Matney[1]; *[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. Paris[1]; James S. Prell[1]; *[1]University of Oregon, Department of Chemistry and Biochemistry, Eugene, OR*

ThP 161 **Proton Affinities of Pipecolic Acid Containing Dipeptides from the Extended Kinetic Method**; J.c. Poutsma[1]; Trinh Ton[1]; Miko Miwa[1]; Laurel Nicks[1]; Katarina Faben[1]; Mark Velasquez[2]; Mark Warren[2]; Jennifer Poutsma[2]; *[1]College of William & Mary, Williamsburg, VA; [2]Old Dominion Univeristy, Norfolk, VA*

ThP 162 **Would building of a true instrument-independent database for product ion spectra in non-resonant mode be a chimera?**; Amandine Hueber[1]; Annelaure Damont[2]; Hanna Kulyk[3]; Martin Green[4]; Ekaterina Darii[5]; Edith Nicol[6]; Sophie Liuu[1]; Denis Lesage[7]; Yves Gimbert[7, 8]; Alain Perret[5]; Gwenaëlle LAVISON-BOMPARD[9]; Yacine Nia[1]; Olivier Firmesse[1]; Jacques Antoine Hennekinne[1]; François Fenaille[2]; Christophe Junot[2]; Justine Bertrand-Michel[10]; Nicolas Cenac[11]; 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,* *France; [4]Waters Corporation, Wilmslow, United Kingdom; [5]Génomique métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry, France; [6]Laboratoire de Chimie Moléculaire, CNRS – IP Paris, Ecole polytechnique, Palaiseau, France; [7]IPCM - Sorbonne Université, UMR CNRS 8232, Paris, France; [8]Département de chimie Moléculaire, UMR CNRS 5250, Université Grenoble Alpes, Grenoble, France; [9]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; [10]I2MC, Université de Toulouse, Inserm, MetaboHub, Toulouse, France; [11]IRSD, Université de Toulouse, INSERM, INRA, INP ENVT, Université de Toulouse 3 Paul Sabatier, Toulouse, France; [12]Emeritus, Morangis, France*

ThP 163 **Gas-phase fragmentation of symmetric and asymmetric viologen-based host-guest complexes**; Daniel M Hristov[1]; Hugo Y. Samayoa-Oviedo[1]; Julia Laskin[1]; *[1]Purdue 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 Lenze[1]; Michael Van Stipdonk[1]; Justin Terhorst[1]; *[1]Duquesne University, Pittsburgh*

ThP 165 **Gas-phase dissociation and thermal decomposition of mono- and di-cation ionic liquids**; Taofiq O Abdulraheem[1]; Amanda Patrick[1]; *[1]Mississippi state university, Starkville, MS*

ThP 166 **Fimsbactin: an Ongoing Theoretical Study of bonding to FeIII Forming Complexes**; Daryl Giblin[1]; Michael L. Gross[2]; Timothy Wencewisz[3]; *[1]Washington University, St Louis, MO; [2]Washington University in St. Louis, St Louis, MO; [3]Washington university in St louis, St Louis, MO*

ThP 167 **Peptide Chain Extension and Chiral Preference Mediated by Oxazolone Intermediate in Aqueous Microdroplets**; Lingqi Qiu[1]; R. Graham Cooks[1]; *[1]Purdue University, WEST LAFAYETTE, IN*

ThP 168 **Spontaneous Prebiotic Condensation Reactions in Impinging Streams of Aqueous Microdroplets**; Dylan T. Holden[1]; Nicolas M. Morato[1]; Myles Q. Edwards[1]; Lingqi Qiu[1]; R. Graham Cooks[1]; *[1]Purdue 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 Bochenek[1]; Addie Keating[1]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH*

ThP 170 **Gas-phase Acidity of D/L-Cysteine-Containing Oligopeptides by Computational and Mass Spectrometry Studies**; Shiyuan Wang[1]; Yuntao Zhang[2]; Jianhua Ren[2]; *[1]University of the Pacific, Stockton, CA; [2]University of The Pacific, Stockton, CA*

ThP 171 **Automated Spectrum Annotation and Structure Disambiguation of Released N-linked Glycans**; Gary Wilson[1]; Anastasia Chernykh[2]; Rebecah Kawahara[2]; St. John Skilton[1]; Morten Thaysen-Andersen[2]; Marshall Bern[1]; *[1]Protein Metrics, LLC, Cupertino, CA; [2]Macquarie University, Sydney, Australia*

ThP 172 **Absolute and relative quantification of bovine milk oligosaccharides using LC-MS based methods**; Yu Wang[1]; Yu-Ping Huang[1]; Sierra Durham[1]; Daniela Barile[1]; *[1]UC 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]; *[1]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; [2]Asia Glycomics Reference Site, Chungnam National University, Daejeon, South Korea*

ThP 174 **Unusual free oligosaccharides found in human, bovine and caprine milk**; Weichien Weng[1]; Chi-Kung Ni[1]; *[1]Institute 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 Wang[1]; Aditya Kulkarni[2]; Kate Yu[2]; Lingjun Li[3]; *[1]University of Wisconsin-Madison, Madison, WI; [2]908 Devices, Boston, MA; [3]School 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]; *[1]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, South Korea; [2]Asia-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 Palomino[1]; David C Muddiman[1]; *[1]North Carolina State University, Raleigh, NC*

ThP 179 **LC-MS/MS Characterization of Glycans in Pig Sertoli Cells to Understand Complement System Behavior**; Andrew I. Bennett[1]; Rachel L. Washburn[2]; Jannette M. Dufour[2]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]Texas Tech University Health Sciences Center, Lubbock, Texas*

ThP 180 **N-linked Glycan quantitation, Is relative quantitation altered by label choice?**; Hoang Kim Ngan Thai[1]; Ron Orlando[1]; *[1]University 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 Ahmadi[1]; Cristian D Gutierrez Reyes[1]; Sherifdeen Onigbinde[1]; Akeem Adeyemi Sanni[1]; Andrew I Bennett[1]; Peilin Jiang[1]; Oluwatosin Daramola[1]; Mojgan Atashi[1]; Vishal Sandilya[1]; Yehia Mechref[1]; *[1]Texas 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 Cherkassky[1]; Chaoshuang Xia[1]; Margaret Downs[1]; Dimitris Papanastasiou[2]; Athanasios Smyrnakis[2]; Pengyu Hong[3]; Catherine E. Costello[1]; Cheng Lin[1]; *[1]Boston University Chobanian and Avedisian School of Medicine, Boston, MA; [2]Fasmatech, NCSR Demokritos, Athens, Greece; [3]Brandeis University, Waltham, MA*

ThP 183 **Field-asymmetry ion mobility spectrometryto improve the separation and identification of released N-glycans**; Denis Morsa[1]; Zoltan Szabo[1]; Cornelia L Boeser[1]; *[1]Thermo 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 it's 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 Enders[1]; Taufika Islam Williams[1]; Kenneth P Garrard[1]; Steven Broome[2]; Rachel Harris[2]; Shahadat Reza[2]; David C Muddiman[1]; *[1]North Carolina State University, Raleigh, NC; [2]MOBILion Systems, Inc, Chadds Ford, PA*

ThP 188 **Improved Hydrophilic Interaction Liquid Chromatography for LC/MS Analysis of Released N-Glycans**; Randall Robinson[1]; Nandini Singh[1]; Andrei Bordunov[2]; Steven Mast[1]; Tom Rice[1]; Aled Jones[1]; Oscar

Potter[2]; [1]*Agilent Technologies, Folsom, CA;* [2]*Agilent Technologies, Santa Clara, CA*

ThP 189 **Serum N-glycans analysis by LC-MS allows the prediction of patients' response to Vedolizumab treatment for Crohn's Disease**; Georgia Elgood-Hunt[1]; Alex Adams[2]; Thomas Sénard[1]; Richard Gardner[1]; Wouter De Jonge[3]; Andrew Li Yim[3]; Alexandra Noble[2]; Jack Satsangi[2]; Vincent Joustra[3]; Geert Dhaens[3]; Daniel Spencer[1]; [1]*Ludger Ltd, Abingdon, United Kingdom;* [2]*Oxford University, Experimental Medicine Division, Oxford, United Kingdom;* [3]*Amsterdam University Medical Center, Inflammatory Bowel Disease Center, Amsterdam, Netherlands*

ThP 190 **Chemoenzymatic Synthesis of Sialylglycosphingosines using One-Pot MultiEnzyme (OPME)**; John Mcarthur[1]; Pierce Carrouth[1]; Katie Miller[1]; Bailey Padgett[1]; Dana Moore[1]; L. Andrew Lee[1]; [1]*IMCS, Irmo, SC*

ThP 191 **D-Va: prediction and interpretation of intact N-glycopeptidetandem mass spectra by deep learning**; Zhewei Liang[1]; Matthew P. Campbell[2]; Richard (DJ) Shipman[1]; Monil Gandhi[1]; Paul Aiyetan[1]; Norton Kitagawa[1]; Daniel Serie[1]; [1]*InterVenn Biosciences, South San Francisco, CA;* [2]*InterVenn 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 Turner[1]; Samuel E. Hoff[2]; Adwaith B. Uday[3]; Algirdas Velyvis[1]; Natalie Zeytuni[3]; Massimiliano Bonomi[2]; Siavash Vahidi[1]; [1]*University of Guelph, Guelph, ON;* [2]*Institut Pasteur, Paris, France;* [3]*McGill University, Montreal, Québec*

ThP 193 **Using Mass Spectrometry Techniques to Capture Mechanosensitivity in Cardiac Proteins**; Elena S Holden[1]; Miranda Collier[1]; Lucia Parolini[1]; Dirk Aarts[1]; Katja Gehmlich[2]; Justin LP Benesch[1]; [1]*University of Oxford, Oxford, United Kingdom;* [2]*University 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 Chow[1]; Cristina Lento[1]; Derek Wilson[1]; [1]*York 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 O Matthew[1, 2]; Rohana Liyanage[1, 2]; Shivakumar Sonnaila[1]; Thallapuranam Krishnaswamy S Kumar[1]; Jackson Lay Jr. [1, 2]; [1]*UNIVERSITY OF ARKANSAS, FAYETTEVILLE, AR;* [2]*Arkansas State-wide mass spectrometry facility, FAYETTEVILLE, AR*

ThP 196 **Establishing HDX-MS and other biophysical approaches to interrogate CC885 mediated GSPT1 degradation**; Shruti Nayak[1]; Paul Tawa[1]; Cory Rice[1]; Michael Eddins[2]; Thierry Fischmann[1]; Li Xiao[1]; Raphaelle Berger[1]; David G. McLaren[1]; Haihong Zhou[1]; [1]*Merck & Co., Inc., Kenilworth, New Jersey;* [2]*Merck & 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; *Genentech, South San Francisco, CA*

ThP 198 **Differentiating Conformational Changes induced by Degraders & Non-degraders in BCL-6 and ERα usingHydrogen Deuterium Exchange Mass Spectrometry (HDX-MS)**; Ekaterina G. Deyanova[1]; Richard Y-C Huang[1, 2]; Robert Langish[1]; Dalia Weiss[3]; Jinyi Zhu[3]; Andy Christoforou[3]; Isabella Tran[3]; Minerva Tran[3]; Veerabahu Shanmugasundaram[4]; Aaron Balog[1]; David Weis[1]; Petia Shipkova[1]; Ingrid Wertz[5, 6]; [1]*Bristol-Myers Squibb, Princeton, NJ;* [2]*Janssen Research & Development, Spring House, PA;* [3]*Bristol-Myers Squibb, San Diego, California;* [4]*Bristol-Myers Squibb, Cambridge, MA;* [5]*Lyterian Therapeutics, San Francisco, California;* [6]*Bristol-Myers Squibb, Brisbane, CA*

ThP 199 **Probing the Effects of Hydrogen-Deuterium Exchange on Protein Stability in Solution and the Gas Phase**; Yousef Haidar[1]; Lars Konermann[2]; [1]*western university, London, ON;* [2]*Western 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. Haynes[1]; Theodore R. Keppel[1]; Sarah Osman[1]; Betlehem Mekonnen[1]; Adrian R. Woolfitt[1]; Yu Zhou[1]; Dongxia Wang[1]; John R. Barr[1]; [1]*Centers 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. Keppel[1]; Christopher A. Haynes[1]; Adrian R. Woolfitt[1]; Sarah H. Osman[1]; Betlehem Mekonnen[1]; Dongxia Wang[1]; John R Barr[1]; [1]*CDC, 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 Ortega[1]; Margot Di Cesare[2]; Jean-Michel Jault[2]; Cédric Orelle[2]; Etienne Meunier[1]; Julien Marcoux[1]; [1]*IPBS Toulouse, Toulouse, France;* [2]*Universite de Lyon, Lyon, France*

ThP 203 **Epitope mapping of polyclonal antibodies in vaccine-elicited human serum**; Mulin Fang[1]; Oliver Wu[1]; Joel B. Langford[1]; Kellye A. Cupp-Sutton[1]; Kenneth Smith[2]; Kathleen Norris[2]; Judith A. James[2]; Si Wu[1]; [1]*University of Oklahoma, Norman, OK;* [2]*Oklahoma Medical Research Foundation, Oklahoma City, OK*

ThP 204 **Hydrogen Deuterium Exchange Mass Spectrometry Reveals Protein Conformational Changes Upon N-terminal PEGylation**; Brent A Kochert[1]; Ross Yang[1]; Hongxia Wang[1]; Hillary A. Schuessler[1]; [1]*Merck & Co., Inc., Kenilworth, New Jersey*

ThP 205 **HDX-MS and XL-MS analyses of antigen-IgG-FcγRIIIa interactions**; Yuki Yamaguchi[1]; Natsumi Wakaizumi[1]; Mine Irisa[1]; Takahiro Maruno[1]; Mari Shimada[1]; Koya Shintani[1]; Haruka Nishiumi[1]; Rina Yogo[2, 3, 4]; Saeko Yanaka[2, 3, 4]; Daisuke Higo[5]; Tetsuo Torisu[1]; Koichi Kato[2, 3, 4]; Susumu Uchiyama[1, 2]; [1]*Osaka Univerisity, Suita, Japan;* [2]*Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Sciences, Okazaki, Japan;* [3]*Institute for Molecular Science (IMS), National Institutes of Natural Sciences, Okazaki, Japan;* [4]*Nagoya City University, Nagoya, Japan;* [5]*Thermo Fisher Scientific, Yokohama, Japan*

ThP 206 **Structural Mass Spectrometry on the Track of Neurodegenerative Diseases**; Petr Man[1, 2]; Zuzana Kalaninova[1, 2]; Sona Galuskova[3]; Tibor Mosko[3]; Michael Volny[1, 2]; Karel Holada[3]; Petr Novák[1, 2]; [1]*BioCeV - Institute of Microbiology, Prague 4, Czech Republic;* [2]*Charles University, Faculty of science, Prague, Czech Republic;* [3]*Charles 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 Kish[1]; Jonathan Phillips[1]; [1]*University 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 Peterle[1]; Nicholas L. Yan[2]; Elena S. Klimtchuk[3]; Thomas E. Wales[1]; Olga Gursky[3]; Gareth J. Morgan[3]; Jeffery W. Kelly[2]; John R. Engen[1]; [1]*Department of Chemistry & Chemical Biology, Northeastern University, Boston, MA;* [2]*Department of Chemistry, The Scripps Research Institute, La Jolla, CA;* [3]*Amyloidosis Center,* *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 Srinivasu[1]; Farah Haque[2, 3]; Radhika Subramanian[2, 3]; John R. Engen[1]; *[1]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA; [2]Department of Molecular Biology, Massachusetts General Hospital, Boston, MA; [3]Department of Genetics, Harvard Medical School, Boston, MA*

ThP 210 **Effect of Osmolytes on WNK Kinases by HDX**; Oladimeji Sunday Olaluwoye[1]; Divyasri Damacharla[2]; Radha Akella[3]; John M Humphreys[3]; Darby Ball[2]; Elizabeth J Goldsmith[4]; Sheena D'arcy[2]; *[1]The University of Texas at Dallas, Richardson, TX; [2]The University of Texas at Dallas, Richardson, Texas; [3]University of Texas Southwestern Medical Center, Dallas, TX; [4]University 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 Morakabi[1]; Noushin Akhavantabib[1]; Darby J Ball[1]; Sheena D'arcy[1]; *[1]The 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 Wong[1]; Wai Po Kong[1]; Pui Kin So[1]; Yu Wai Chen[1]; Zhongping Yao[1]; *[1]The Hong Kong Polytechnic University, Kowloon, Hong Kong*

ThP 213 **Ligand-induced conformational changes on β1-Adrenergic Receptor coupled to miniGs mapped by Hydrogen-Deuterium Exchange Mass Spectrometry**; Joanna Toporowska[1]; Parth Kapoor[2]; Jonathan Hopper[2]; Argyris Politis[1, 3]; *[1]King's College London, London, United Kingdom; [2]OMass Therapeutics, Oxford, United Kingdom; [3]University 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 Zhang[1]; Tsz-Fung Wong[1]; Pui-Kin So[1]; Zhongping Yao[1]; *[1]The Hong Kong Polytechnic University, Kowloon, Hong Kong*

ThP 215 **Structural characterization of p97/VCP AAA+ ATPase via Hydrogen-Deuterium Exchange Mass-Spectrometry**; Ezgi Basturk[1]; Baran Dingiloglu[1]; Berfin Dogan[1]; Gizem Dinler Doganay[1]; *[1]Istanbul Technical University, Istanbul, Turkey*

ThP 216 **Mapping Allosteric Regulation of Pyruvate Kinases by Native and Synthetic Ligands**; Evan Bonnand[1]; Agnieszka Bogucka[2]; Marko Hyvönen[2]; Sheena D'arcy[1]; *[1]UT Dallas, Richardson, TX; [2]University 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-Lukaszewska[1]; Qi Huang[2]; Luke Berry[3]; Hayden Kallas[4]; John Peters[5]; Lance Seefeldt[4]; Simone Raugei[2]; Brian Bothner[1]; *[1]Montana State University, Bozeman, MT; [2]PNNL, Richland, WA; [3]MSU; BOZEMAN, MT, Bozeman, MT; [4]Utah State University, Logan, UT; [5]University 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 Du[1]; Igor A Kaltashov[1]; *[1]University of Massachusetts-Amherst, Amherst, MA*

ThP 219 **Mechanism of complement cascade activation probed with HDX-MS**; Charles Mundorff[1]; Michael Watson[1]; Lauren Carter[1]; Malika R Hale[1]; Adian Valdez[1]; David J Rawlings[1]; Marion Pepper[1]; Neil King[1]; Miklos Guttman[1]; *[1]University of Washington, Seattle, WA*

ThP 220 **Determination of antibody epitopes against Sars-CoV2 antigens using Hydrogen Deuterium Exchange- Mass Spectrometry**; Ankit P Jain[1]; Liu Xu[1]; Filipp Frank[1]; Wilbur Lam[1, 2, 3, 4]; Eric Ortlund[1]; Blaine Roberts[1]; *[1]Emory School of Medicine, Emory University, Atlanta, GA; [2]Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology & Emory University, Atlanta, GA; [3]Aflac Cancer and Blood Disorders Center of Children's Healthcare of Atlanta, Atlanta, GA; [4]Pediatric 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. Petrotchenko[1]; Roopa Thapar[2]; Edith Nagy[2]; Jason B. Cross[2]; Christoph H. Borchers[1, 3, 4, 5]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [2]M.D. Anderson Cancer Center, Institute for Applied Cancer Science, Therapeutics Discovery Division, Houston, TX; [3]Gerald Bronfman Department of Oncology, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [4]Division of Experimental Medicine, McGill University, Montreal, QC; [5]Department 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 Rojas[1]; Kevin Jeanne Dit Fouque[2]; Miguel Santos Fernandez[2]; Francisco Alberto Fernandez Lima[2]; *[1]Florida International University, miami, FL; [2]Florida International University, Miami, FL*

ThP 223 **HDX-MS reveals novel aspects of PI3KC2b regulation by its extended N-terminus**; Gillian Leigh Dornan[1]; Klara Haas[1]; Volker Haucke[1]; *[1]Leibniz-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 Papanastasiou[1]; Amanda L Waterbury[2]; Hui Si Kwok[2]; Ceejay Lee[2]; Allyson M Freedy[2]; Cindy Su[2]; Will Hawkins[1]; Andrew Reiter[1]; Samuel M Hoenig[2]; Michael E Vinyard[2]; Brian B Liau[2]; Steven A Carr[1]; *[1]Broad Institute, Cambridge, MA; [2]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA*

ThP 225 **Hydrogen/Deuterium Exchange of a Polyketide Synthase During Its Catalytic Cycle**; Josh Salem[1]; Rebecca Taylor[2]; Kristina Hakansson[2]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Michigan-Ann Arbor, Ann Arbor, MI*

ThP 226 **Mapping interactions of staph enterotoxin B in neutralizing serum**; Clint Vorauer[1]; Camila Boniche-Alfaro[2]; Bettina Fries[2]; Mike Guttmann[1]; *[1]University of Washington, Seattle, WA; [2]Stony 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 Anand[1]; Varun Venkatakrishnan[1]; Sean Braet[1]; *[1]The 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 Hou[1]; Dandan Si[1]; Zhimin Long[2]; Lihai Guo[1]; *[1]SCIEX, Beijing, China; [2]SCIEX, Shanghai, China*

ThP 229 **SP3-enabled high coverage multiplexed cysteine chemoproteomics**; Flowreen Shikwana[1]; Alexandra C. Turmon[1]; Miranda Villanueva[1]; Cindy Truong[1]; Keriann Backus[1]; *[1]UCLA, 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 Wilson[2]; *[1]Medical Proteome-Center, Ruhr-University, Bochum, Germany; [2]Protifi, LLC, Fairport, NY*

ThP 231 **High-throughput label-free opioid receptor binding assays using automated desorption electrospray ionization mass spectrometry (DESI-MS)**; Yunfei Feng[1]; Nicolas M. Morato[1]; Kai-Hung Huang[1]; R. Graham Cooks[1]; *[1]Purdue University, WEST LAFAYETTE, IN*

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aminopeptidase; Leonie Mueller[1]; Simon Peace[2]; Melanie Leveridge[3]; Matthias Trost[1]; Rachel Peltier-Heap[4]; Maria Emilia Dueñas[1]; *[1]Newcastle University, Newcastle upon Tyne, United Kingdom; [2]GSK, Medicinal Chemistry, Stevenage, United Kingdom; [3]GSK, Screening, Profiling and Mechanistic Biology, Stevenage, United Kingdom; [4]GSK, Discovery Analytical, Stevenage, United Kingdom*

ThP 233 **Automated Data Analysis and Robust Quality Control for Affinity Selection Mass Spectrometry**; Matthew Green[1]; Juan Florez[2]; Malwina Michalak[3]; Stephan Steigele[2]; Stephan Heyse[2]; *[1]Genedata, Cambridge, United Kingdom; [2]Genedata, Basel, Switzerland; [3]Genedata, Munich, Germany*

ThP 234 **Untargeted LC-MS metabolomics screening of 500,000 serum samples identifies novel biomarkers for cancer, cardiovascular, and liver diseases**; Boris Sarvin[1]; Mark Vernik[1]; Avi Shoshan[1]; Eldad Kepten[1]; Carmel Shor[1]; Ori Kronfeld[1]; Avishai Gavish[1]; Shira Shaham-Niv[1]; Tomer Shlomi[1, 2]; *[1]MetaSight Diagnostics LTD, Rehovot, Israel; [2]Faculty 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 Pu[1]; Andrew Radosevich[1]; Omprakash Nacham[1]; James Sawicki[1]; Nari Talaty[1]; Scott Ugrin[1]; Sujatha Gopalakrishnan[1]; Jon Williams[1]; Nathaniel Elsen[1]; *[1]AbbVie Inc., North Chicago, IL*

ThP 236 **Acoustic Ejection Mass Spectrometry for Ultrahigh-Throughput Analysis of Pharmaceutical Targets**; Hang Hu[1]; Ophelia Ukaegbu[1]; Joseph Gouker[1]; Stephanie Chun[1]; Wai Ling Cheung-Lee[1]; Karla Camacho Soto[1]; Hsing-I Ho[1]; Amanda Marie Makarewicz[1]; Stephanie Galanie[1]; Xiujuan Wen[2]; David G. McLaren[2]; Kevin P. Bateman[3]; Chang Liu[4]; Thomas R. Covey[4]; Erik L. Regalado[1]; Emmanuel Appiah-Amponsah[1]; *[1]Merck & Co., Inc., Rahway, NJ; [2]Merck & Co., Inc., Kenilworth, NJ; [3]Merck & Co., Inc., West Point, PA; [4]SCIEX, Concord, ON*

ThP 237 **High throughput characterization of polyamide hydrolase activity using open port sampling interface mass spectrometry**; John F. Cahill[1]; Vilmos Kertesz[1]; Patricia Saint-Vincent[1]; Hannah Valentino[1]; Erin Drufva[1]; Joshua K. Michener[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN*

ThP 238 **A rapid workflow for high-throughput FFPE-based proteomics**; Ganesh Pujari[1]; Kiran Mangalaparthi[1]; M. Cristine Charlesworth[1]; Benjamin Madden[1]; Amy Josephine French[1]; Gunveen Sachdeva[1]; Eugenio Daviso[2]; Ulrich Thomann[2]; Patrick McCarthy[2]; Sameer Vasantgadkar[2]; Deb Bhattacharyya[2]; Akhilesh Pandey[1]; *[1]Mayo Clinic, Rochester, Minnesota; [2]Covaris, Lexington, MA*

ThP 239 **Building spectral libraries to enable large-scale quantitative proteomic studies in human plasma**; Jian Wang[1]; Harendra Guturu[1]; Yingxiang Huang[1]; Seth Just[1]; Shadi Ferdosi[1]; Xiaoyan Zhao[1]; Andrew Nichols[1]; Lee S Cantrell[1]; Alexey Stukalov[1]; Iman Mohtashemi[1]; Ting Huang[1]; Lucy Williamson[1]; Gabriel Castro[1]; Eltaher Elgierari[1]; Ryan W. Benz[1]; Khatereh Motamedchaboki[1]; Daniel Hornburg[1]; Asim Siddiqui[1]; Serafim Batzoglou[1]; *[1]Seer, Inc., Redwood City, CA*

ThP 240 **Rapid Characterization of Unpurified Biotherapeutics through Online Buffer Exchange**; Michael Poltash[1]; Weijing Liu[2]; Elsa Gorre[1]; Scott Kronewitter[2]; Rosa Viner[2]; Andrew Mahan[1]; Hirsh Nanda[1]; *[1]Janssen Pharmaceuticals, Spring House, PA; [2]Thermo Fisher Scientific, San Jose, California*

ThP 241 **High-throughput proteomics on a novel high-resolution accurate mass (HRAM) platform**; Tabiwang N. Arrey[1]; Daniel Hermanson[2]; Jeff Op De Beeck[3]; Runsheng Zheng[4]; Xuefei Sun[5]; Paul Jacobs[3]; Nicolaie Eugen Damoc[1]; Vlad Zabrouskov[2]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Thermo Fisher Scientific, San Jose, California; [3]Thermo Fisher Scientific - Belgium, Ghent, Belgium; [4]Thermo Fisher Scientific, Germering, Germany; [5]Thermo 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 Burton[1]; Justin T Munro[2]; Michelle Pemberton[1]; Julie Quayle[1]; Joseph Kozole[2]; Roland Annan[2]; *[1]Discovery Analytical, Screening, Profiling, and Mechanistic Biology, GlaxoSmithKline, Stevenage, United Kingdom; [2]Discovery 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. Dziekonski[1]; Thomas C. Sams[1]; Lucas J. Szalwinski[1]; L. Edwin Gonzalez[1]; R. Graham Cooks[1]; *[1]Purdue 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-Aliste[1]; Jennifer Aguilan[1]; Simone Sidoli[1]; *[1]Albert Einstein College of Medicine, Bronx, NY*

ThP 246 **Ion pre-accumulation in bent flatapole boosts MS2 sensitivity and peptide identifications in an Orbitrap Exploris 480 mass spectrometer**; Florian Harking[1]; Julia Kraegenbring[2]; Hamish Stewart[2]; Pedro Navarro[2]; Konstantin Ayzikov[2]; Dmitry Grinfeld[2]; Alexander Harder[2]; Alexander Makarov[2]; Jesper Velgaard Olsen[1]; *[1]NNF CENTER FOR PROTEIN RESEARCH, Copenhagen, Denmark; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 247 **Quantification of Terpenes with Rapid "Shotgun" APGC-IMS-MS**; Jeffrey Morre[1]; Sam Bassett[2]; Claudia Maier[2]; Jan F. Stevens[2, 3]; *[1]Oregon State University, Corvallis, OR; [2]Oregon State University, Corvallis; [3]Global Hemp Innovation Center, Corvallis, OR*

ThP 248 **Multi-omic Analyses Enabled by Microchip Capillary Electrophoresis and Trapped Ion Mobility Mass Spectrometry**; Zhan Gao[1]; Melissa R. Pergande[1]; Matthew S Fischer[1]; Eli J Larson[1]; Morgan Mann[1]; Kevin M. Buck[1]; Jake A Melby[1]; Yanlong Zhu[1]; Adi M Kulkarni[2]; J. Will Thompson[2]; Guillaume Tremintin[3]; Kate Yu[2]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]908 Devices, Inc., Boston, MA; [3]Bruker Daltonics, San Jose, CA*

ThP 249 **Operating the Omnitrap Platform in Data-Dependent Acquisition Mode: Electron Induced and Electron Capture Dissociation of BSA and HeLa Digests**; Mariangela Kosmopoulou[1]; Athanasios Smyrnakis[1]; George Alevizos[1]; Dimitris Papanastasiou[1]; *[1]Fasmatech, NCSR Demokritos, Athens, Greece*

ThP 250 **High-throughput metabolic screening using neutron encoded 96-plex tags**; Michael R Armbruster[1]; Scott F Grady[1]; Christopher K Arnatt[1]; James L Edwards[1]; *[1]Saint Louis University, St. Louis, MO*

ThP 251 **High-Depth Multiplexed Drug Profiling with the Orbitrap Ascend**; Steven R. Shuken[1]; Graeme C. McAlister[2]; William D. Barshop[2]; Jesse D. Canterbury[2]; David Bergen[2]; Jingjing Huang[2]; Romain Huguet[2]; Joao A. Paulo[1]; Amanda E Lee[2]; Vlad Zabrouskov[2]; Steven P Gygi[1]; Qing Yu[1]; *[1]Department of Cell Biology, Harvard Medical School, Boston, MA; [2]Thermo 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 Simchuk[1]; Andrew D. Mesecar[2]; Mackenzie E Chapman-Imhoff[2]; Richard Van Breemen[3]; *[1]Oregon State University, Corvallis, OR; [2]Purdue University, WEST LAFAYETTE, IN; [3]Oregon State University, Corvallis*

ThP 253 **High-throughput bioanalysis of adenosine by LS-I-LC-MS/MS platform**; Yuanqiang Su[1]; Ke Song[1]; Xiaotong Li[1]; Xinxin Wen[1]; Juezhu Fan[1]; Cheng Chen[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; *[1]WuXi AppTec, Shanghai, China*

ThP 254 **Subcellular Resolution Biochemical Imaging Method Combining Electron Microscopy with Vacuum Electrospray Beams**; John Sentmanat[1]; Peter A Kottke[1]; Andrei G Fedorov[1]; *[1]Georgia Institute of Tchnology, 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 Joignant[1]; David C Muddiman[1]; *[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 Claude[1]; William Johnson[1]; Joel Keelor[2]; Emma Marsden-Edwards[1]; Martin Palmer[1]; *[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 Friedrich[1]; Ingela Lanekoff[1]; *[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 Hirotani[1]; Hisanao Hazama[1]; Kunio Awazu[2]; *[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-Grimaudo[1]; Lex Pillatsch[1]; James Whitby[1]; Michael Grössl[1]; Steffen Bräkling[1]; *[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 Dufresne[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 Battle[2]; Yuchen Xiang[2]; Stefania Maneta-Stavrakaki[2]; Lauren Ford[2]; Robert T Murray[2]; Josephine Bunch[3]; 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 Dreisbach[1]; Carolin M Morawietz[2]; Karl Christian Schäfer[1]; Kerstin Strupat[3]; 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 Spengler[3]; Sabine Schulz[3]; Julian Schneemann[3]; Karl-Christian Schäfer[4]; *[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 West[1]; Joshua Fischer[1]; Corinna Henkel[2]; Gargey B. Yagnik[3]; Mark Lim[3]; *[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 Ouyang[1]; Xiangyu Gu Guo[1]; Aojie Zhang[1]; Zhijun Cai; Wenpeng Zhang[1]; *[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 Jia[1]; Anya Eyres[1, 3]; Natasha Smith[1]; Michael Burt[1]; Josephine Bunch[2, 3]; Zoltan Takats[2, 4]; Mark Brouard[1]; Felicia M Green[2]; *[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 Barnette[1]; Richard Beger[1]; Pravin R. Kaldhone[1]; Joseph Hanig[2]; J. Edward Fisher[2]; Dan Mellon[2]; Grace Lee[3]; Amy Inselman[1]; E. Ellen Jones[1]; *[1]National Center for Toxicological Research, Jefferson, AR; [2]Center for Drug Evaluation and Research, Silver Spring, MD; [3]Elevar 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 Jang[1]; Hyeyeon Kang[1]; Boyoung Lee[1]; *[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 Siciliano[1]; Laura Brunelli[1]; Giulia De Simone[1]; Aurelia Morabito[1]; Francesca Pischiutta[1]; Federico Moro[1]; Elisa R. Zanier[1]; Roberta Pastorelli[1]; Enrico Davoli[1]; *[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 Butrico[3]; Elizabeth K Neumann[1, 4]; Madeline E Colley[1, 4]; Katherine N GIbson-Corley[3]; Lukasz G Migas[5]; Raf Van De Plas[5]; 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 Tuck[1]; Florent Grélard[1]; Landry Blanc[1]; Véronique Dartois[2]; Nicolas Desbenoit[1]; *[1]Université de Bordeaux, Bordeaux, France; [2]Hackensack Meridian Health Center for Discovery & Innovation, Nutley, NJ*

ThP 274 **Laser ablation inductively coupled plasma mass spectrometry imaging reveals how gold nanoparticle surface charge influences their distribution and excretion pathways**; Jeerapat Doungchawee[1]; Laura J Castellanos[1]; Kristen Sikora[1]; Xianzhi Zhang[1]; Yuanchang Liu[1]; Vincent M. Rotello[1]; Richard W. Vachet[1]; [1]*University 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. Cousineau[1]; Mohammed H. Sarikahya[1]; Marta De Felice[1]; Aleksandra Doktor[1]; Steven R. Laviolette[1]; Daniel B. Hardy[1]; Ken K.-C. Yeung[1]; [1]*University of Western Ontario, London, ON*

ThP 276 **Spatiotemporal Profiling of the Lipidome, Proteome, and Phosphoproteome of PLK1 Inhibited Colorectal Cancer Spheroids**; Emily R. Sekera[1]; Brian D. Fries[1]; Amanda B. Hummon[1]; [1]*The Ohio State University, Columbus, OH*

ThP 277 **Visualizing the spatial distribution of flavonoids and phenolic acids in the tuber root of Tetrastigma hemsleyanum using AP-MALDI-MSI**; Junling Dun[1]; Hongyuan Hao[1]; Taohong Huang[1]; Yan Lin[2]; [1]*Shimadzu (China) Co., Ltd.,, Shanghai, China;* [2]*Tongde Hospital of Zhejiang Province, Hangzhou, China*

ThP 278 **Mass Spectrometry Imaging Studies of Metabolites In Mice Heart Affected With Chagas Disease**; Dan Chen; *Univerity of Oklahoma, department of chemistry and bochemistry, 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]; [1]*UW-Madison School of Pharmacy, Madison, WI;* [2]*Department of Urology, University of Wisconsin-Madison, Madison, WI;* [3]*George M. O'Brien Center, University of Wisconsin-Madison, Madison, WI;* [4]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI;* [5]*Department 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 Chen[1]; Kaoru Nakagawa[2]; Jian Su[3]; Keisuke Shima[1]; Yongli Liu[3]; Rong Lei[3]; Jing Dong[1]; Hao Yuan[3]; Xiaolei Wang[3]; Satoshi Kasamatsu[4]; Lei Cao[1]; Xiaodong Li[1]; [1]*Shimadzu China Innovation Center, Beijing, China;* [2]*Healthcare Solution Unit, Solutions Center of Excellence, Shimadzu Corporation, Kyoto, Japan;* [3]*Hebei Institute for Drug and Medical Device Control, Shijiazhuang, China;* [4]*MS 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 Ebbini[1]; Hua Zhang[1]; Peng-Hsuan Huang[2]; Lingjun Li[1, 2]; [1]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI;* [2]*Department 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 Verbeeck[1]; Maria José Q Mantas[1]; Eylan Yutuc[2]; Alice Ly[1]; William J Griffiths[2]; Marc Claesen[1]; Yuqin Wang[2]; [1]*Aspect Analytics, Genk, Belgium;* [2]*Swansea 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 Ye[1]; Ruijun Jian[2]; Wenpeng Zhang[1]; Yu Xia[2]; Ouyang Zheng[1]; [1]*Tsinghua University, Beijing, China;* [2]*Tsinghua 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 Yang[1]; Azad Eshghi[1]; Amy Li[2]; Libin Xu[2]; Shannon Cornett[1]; [1]*Bruker Daltonics, Billerica, MA;* [2]*University of Washington, Seattle, WA*

ThP 286 **MALDI Mass Spectrometry Imaging of 13C6-Glucose Uptake Measured in TCA Metabolites from Glioblastoma Mouse Brain**; Joshua L Fischer[1]; Kari Wilder-Romans[2]; Ethan Yang[1]; Savannah R Snyder[1]; Katherine Stumpo[1]; Angelica Lin[2]; Zitong Zhao[2]; Jie Xu[2]; Daniel R. Wahl[2]; [1]*Bruker Daltonics, Billerica, MA;* [2]*University 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 Gitta[1]; Eva Szabo[1]; Laszlo Mark[1]; [1]*Institute 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 Zerebinski[1]; Joshua Soto-Ocaña[2]; Jonathan T. Specker[1]; Joseph P. Zackular[2, 3]; Boone M. Prentice[1]; [1]*University of Florida, Chemistry Department, Analytical Chemistry Division, Gainesville, FL;* [2]*Division of Protective Immunity, Children's Hospital of Philadelphia, Philadelphia, Pennsylvania;* [3]*Department 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 Towers[1]; Lisa Reid[1]; Joanne Ballantyne[1]; Alicia Rosell-Hidaglo[2]; Kirsten Headspith[2]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*Cyprotex 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 Uhlmansiek[1]; Andrew E Paulson[1]; Young-Jin Lee[1]; [1]*Iowa 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 Bailey[1]; Catia D S Costa[1]; Janella M De Jesus[2]; Josephine Bunch[2]; [1]*University of Surrey, Guildford, United Kingdom;* [2]*National 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 Andrews[1]; Aleksandra Ogurtsova[2]; Mike Mikula[2]; Ogechi Nwankwoala[2]; Liz Engle[2]; Carole Fakhry[2]; R. Alex Harbison[2]; Maureen Kane[1]; [1]*University of Maryland School of Pharmacy, Baltimore, MD;* [2]*Johns 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 Wadsworth[2]; C. Linn Cadieux[2]; Caitlin M. Tressler[3]; [1]*Oak Ridge Institute of Science Education, Oak Ridge, TN;* [2]*U.S. Army Medical Research Institute of Chemical Defense, Gunpowder, Maryland;* [3]*Johns 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. Migas[4]; Audra M. Judd[1, 3]; Jamie L. Allen[1, 3]; Raf Van De Plas[4]; Jeffrey M. Spraggins[1, 2, 3]; [1]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN;* [2]*Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN;* [3]*Department of Biochemistry, Vanderbilt University, Nashville, TN;* [4]*Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands*

ThP 295 **Multilevel human secondary lymphoid immune system compartmentalization revealed by complementary multiplexing and mass spectrometry imaging**; Benjamin L. Oyler[1]; Jeferson Valencia-Davila[2]; Eirini Moysi[2]; Adam Molyvdas[2]; Kalliopi Ioannidou[3]; Kylie March[2]; David Ambrozak[2]; Laurence De Leval[3]; Giulia Fabozzi[2]; Amina Woods[2]; Richard Koup[2]; Constantinos Petrovas[3]; *[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 Stolley[1]; Natalie Fowlkes[1]; Maria Sophia Stenkamp[1]; Erin H Seeley[2]; Erik Cressman[1]; *[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. Pearce[1]; Neil A. Cross[2]; Laura M. Cole[2]; David P. Smith[2]; James I. Langridge[3]; Emmanuelle Claude[3]; Lucy E. Flint[4]; Richard Goodwin[4]; Malcolm R. Clench[2]; *[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. Bhat[1]; Nancy Milam[1]; 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 Yakobi[1]; Elka Touitou[1]; Hiba Natsheh[1]; Katy Margulis[1]; *[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 Wu[1]; Franklin E. Leach III[1]; *[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 Chatterjee[3]; Nasiruddin Shaikh[3]; Madhuri Gupta[1, 2]; Konstantin Novoselov[1]; Eugene Moskovets[1]; Kaushik Banerjee[3]; Nivedita Bhattacharya[1, 2]; Venkateswarlu Panchagnula[1]; *[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 Claude[1]; Wei Rao[1]; Laurent Bultel[2]; Noelle Elliott[3]; Tristan Renaud[2]; Joanne B Ballantyne[1]; *[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 Xiang[1]; Andrey Liyu[1]; Yumi Kwon[1]; Dehong Hu[1]; William Chrisler[1]; Sarah Williams[1]; Dušan Veličković[1]; Lye Meng Markillie[1]; Ljiljana Paša-Tolić[1]; Ying Zhu[2]; *[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 Kwon[1]; Sarah M Williams[1]; Jing Chen[2]; Geremy C Clair[1]; Dehong Hu[1]; Lye Meng Markillie[1]; Andrey V Liyu[1]; Karl K Weitz[1]; Ronald J Moore[1]; Ernesto S Nakayasu[1]; Martha Campbell-Thompson[2]; Clayton Mathews[2]; Ying Zhu[1, 3]; Wei-Jun Qian[1]; *[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 Rose[1]; Kevin Titeca[1]; Sergii Mamedov[1]; Lucas Maciel Vieira[1]; 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, BioInnovation Institute, Copenhagen, Denmark*

ThP 307 **Tumor heterogeneity of glioblastoma analyzed via SpatialOMx and HiPLEX-IHC MALDI Imaging**; Corinna Henkel[1]; Signe Frost Frederiksen[1]; Katherine A. Stumpo[2]; Matthias Szesny[1]; Jörg W. Bartsch[3]; 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 Ge[1]; Srinivas Koutarapu[1]; Durga Jha[1]; 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 Ridge[1]; Elizabeth K. Neumann[1]; *[1]UC Davis, Davis, CA*

ThP 310 **Large-Scale Interlaboratory Comparison of Imaging Mass Spectrometry Protocols for Spatial Untargeted Metabolomics**; Veronika Saharuka[1]; Måns Ekelöf[1]; Lachlan Stuart[1]; Lucas M. Vieira[1]; Martijn R Molenaar[1]; Alberto Bailoni[1]; Katja Ovchinnikova[2]; Tobias Bausbacher[3]; Dennis Jakob[4]; Mary King[5]; Max Müller[6]; Crystal Pace[7]; Fernanda E. Pinto[8]; Nicole Strittmatter[9]; Jens Soltwisch[10]; Dušan Veličković[11]; Janina Oetjen[12]; Christopher Anderton[11]; Livia

S. Eberlin[13]; Richard Goodwin[9]; Christian Janfelt[8]; Manuel Liebeke[4]; David C. Muddiman[7]; Bernhard Spengler[6]; Klaus Dreisewerd[10]; Carsten Hopf[3, 14, 15]; Theodore Alexandrov[1, 16, 17, 18]; *[1]Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany; [2]Department for BioMedical Research, University of Bern, Bern, Switzerland; [3]CeMOS - Center for Mass Spectrometry and Optical Spectroscopy, Mannheim, Germany; [4]Max Planck Institute for Marine Microbiology, Bremen, Germany; [5]University of Texas at Austin, Austin, TX; [6]Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Gießen, Germany; [7]Department of Chemistry, North Carolina State University, Raleigh, NC; [8]Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark; [9]AstraZeneca, Cambridge, United Kingdom; [10]Institute of Hygiene, University of Münster, Münster, Germany; [11]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington; [12]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [13]Department of Surgery, Baylor College of Medicine, Houston, TX; [14]Medical Faculty of Heidelberg University, Heidelberg, Germany; [15]Mannheim Center for Translational Neuroscience (MCTN), Medical Faculty Mannheim, Heidelberg University, Mannheim, Germany; [16]Metabolomics Core Facility, Heidelberg, Germany; [17]Molecular Medicine Partnership Unit, Heidelberg, Germany; [18]Bio 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. Hale[1]; Tyler R. Wells[2]; Richard J. Mead[2]; Helen J. Cooper[1]; *[1]University of Birmingham, Birmingham, United Kingdom; [2]Sheffield 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. Lu[1]; Hua Zhang[2]; Gargey B. Yagnik[3]; Mark J. Lim[3]; Kenneth J. Rothschild[3]; Andrew J. Schneider[4, 5]; Luigi Puglielli[4, 5]; Lingjun Li[1, 2]; *[1]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [2]University of Wisconsin-Madison School of Pharmacy - Madison, WI, Madison, WI; [3]AmberGen, Inc., Billerica, MA; [4]University of Wisconsin-Madison, Department of Medicine, Madison, WI; [5]Waisman 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 Vandergrift[1]; Kevin J Zemaitis[1]; Arunima Bhattacharjee[1]; Dušan Veličković[1]; Jessica K Lukowski[1]; Ljiljana Paša-Tolić[1]; William Kew[1]; Christopher Anderton[1]; *[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington*

ThP 314 **Novel Myc-driven metabolic vulnerability identified by multimodal mass spectrometry imaging**; Peter Kreuzaler[1]; Paolo Inglese[2]; Avinash Ghanate[1]; Ersa Gjelaj[1]; Vincen Wu[3]; Yulia Panina[1]; Andres Mendez-Lucas[1]; Catherine MacLachlan[1]; Neill Patani[1]; Catherine B Hubert[1]; Helen Huang[3]; Gina Greenidge[4]; Oscar M Rueda[5]; Adam J Taylor[4]; Evdoxia Karali[6]; Emine Kazanc[3]; Amy Spicer[1]; Wei Lin[1]; Daria Thompson[1]; Mariana Silva Dos Santos[1]; Enrica Calvani[1]; Nathalie Legrave[1]; James K Ellis[1]; Rory T Steven[7]; Wendy Greenwood[5]; Mary Green[1]; Emma Nye[1]; Emma Still[1]; Simon T Barry[8]; Richard J A Goodwin[8]; Alejandra Bruna[6]; Carlos Caldas[5]; James Macrae[1]; Luiz Pedro Sorio de Carvalho[1]; George Poulogiannis[6]; Greg McMahon[4]; Zoltan Takats[3]; Josephine Bunch[4]; Mariia Yuneva[1]; *[1]The Francis Crick Institute, London, United Kingdom; [2]Imperial College London, London, United Kingdom; [3]Imperial College London, London, United Kingdom; [4]National Physical Laboratory, Teddington, United Kingdom; [5]University of Cambridge, Cambridge, United Kingdom; [6]The Institute of Cancer Research, London, United Kingdom; [7]National Physical Laboratory, London, United Kingdom; [8]AstraZeneca, Cambridge, United Kingdom*

ThP 315 **Mobility-Modulated Sequential Dissociation of Multiple Precursors (SDIMP) for Highly Multiplexed MS/MS Imaging**; Yao Qian[1]; Xiaoxiao Ma[1]; Zheng Ouyang[1]; *[1]Department 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; *University 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 Migas[5]; 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]; *[1]Mass Spectrometry Research Center, Vanderbilt University,, Nashville, TN; [2]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Pathology, Microbiology, and Immunology, Vanderbilt University Medical Center, 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 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 Leow[1]; Xiaowei Lu[1]; Marc Bosse[1]; Richard R Drake[2]; Peggi M. Angel[2]; Sean Bendall[1]; Mike Angelo[1]; *[1]Stanford University, Stanford, CA; [2]Medical University of South Carolina, Charleston, SC*

ThP 319 **Exploring MALDI-MSI with Higher Metabolite Coverage and Its Application in Spatial Metabolomics**; Jia Yi[1]; Joe L. Rowles[1]; Leah P. Shriver[1]; Gary J. Patti[1]; *[1]Washington 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 Huo[1]; Min Ma[2]; Shuo Qian[2]; Ming Zhang[1]; Jie Pu[1]; Xiaoyu Zhu[1]; Sailee Rasam[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell Park Comprehensive Cancer Institute, Buffalo, NY*

ThP 321 **Aberrant Lipid Metabolism in the Orthotopic Mouse Glioma: A MALDI-MS Imaging and Lipidomic Study**; Hay-Yan J Wang[1]; Chiung-Yin Huang[2, 3]; Kuo-Chen Wei[2, 3, 4, 5]; Kuo-Chen Hung[6]; *[1]National Sun Yat-Sen University, Kaohsiung City, Taiwan; [2]Neuroscience Research Center, Chang Gung Memorial Hospital, Taoyuan, Taiwan; [3]Department of Neurosurgery, New Taipei Municipal TuCheng Hospital, New Taipei City, Taiwan; [4]Department of Neurosurgery, Chang Gung Memorial Hospital, Taoyuan, Taiwan; [5]School of Medicine, Chang Gung University, Taoyuan, Taiwan; [6]Department 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 Okamura[1]; Shinichi Yamaguchi[2]; Takushi Yamamoto[2]; Ryo Inoue[3]; Laura Yuriko González – Teshima[4]; Keisuke Hakamada[4]; Kisaki Amemiya[5]; Kenji Minatoya[4]; Hidetoshi Masumoto[4]; Satoru Noguchi[6]; Ichizo Nishino[6]; Hatsue Ueda[5, 7]; Masaya Ikegawa[1]; *[1]Department of Life and Medical Systems, Doshisha University, Kyotanabe-city, Japan; [2]Shimadzu Corporation, Kyoto-city, Japan; [3]Faculty of Agriculture, Setsunan University, Hirakata-city, Japan; [4]Department of*

Cardiovascular Surgery, Graduate School of Medicine, Kyoto University, Kyoto-city, Japan; [5]Department of Pathology, National Cerebral and Cardiovascular Center, Suita-city, Japan; [6]Department of Neuromuscular Research, National Center of Neurology and Psychiatry, Kodaira-city, Japan; [7]Department 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 Saunders[1]; Holly-May Lewis[1]; Catia Costa[1, 2]; Johanna Von-Gerichten[1]; Priyanka Gupta[3]; Eirini Velliou[3]; Melanie Bailey[1]; *[1]University of Surrey, Guildford, United Kingdom; [2]Surrey Ion Beam Centre, Guildford, United Kingdom; [3]University 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 Wu[1]; Muthu K. Shanmugam[1]; Pakkiri Leroy Sivappiragasam[1]; H. Ling Lieng[1]; Hyungwon Choi[1]; Eugene Goh[1]; Li Ling Tan[2]; Yoon Sim Yap[3]; Soo Chin Lee[4]; A. Mark Richards[1]; Chester L. Drum[1]; *[1]National University of Singapore, Singapore, Singapore; [2]National University Heart Centre, Singapore, Singapore; [3]Department of Medical Oncology at National Cancer Centre Singapore, Singapore, Singapore; [4]National University Cancer Institute, Singapore, Singapore*

ThP 325 **GraphCCS: Prediction of Collision Cross-Section for Metabolites Using Graph Neural Network**; Hsin-Hsiang Chung[1]; Cheng-Chih Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei City, Taiwan*

ThP 326 **Automated and interpretable machine learning for MS metabolomics: predicting cancer diagnosis**; Olatomiwa O Bifarin[1]; Facundo M Fernandez[1]; *[1]Georgia 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 Koelmel[1]; Paul Stelben[1]; Bernard Brooks[2, 3]; Jung Suh[4]; Mark Sartain[5]; Timothy J. Garrett[6]; John A. Bowden[6]; Emma E Rennie[5]; Krystal J Godri Pollitt[1]; *[1]Yale University, New Haven, CT; [2]Innovative Omics, Sarasota, FL; [3]Mudai Studios, Sarasota, FL; [4]Denali Therapeutics, San Francisco, CA; [5]Agilent Technologies, Santa Clara, CA; [6]University of Florida, Gainesville, FL*

ThP 328 **Untargeted exometabolomics of a fast-growing cyanobacterium Synechococcus elongatus PCC11801 strain in different growth media**; Virmal S. Jain[1]; Meghna Srivastava[1]; Prajval Nakrani[2]; Pramod P. Wangikar[1, 2]; *[1]Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai, India; [2]Clarity Bio Systems India Pvt Ltd, Pune, India*

ThP 329 **Plasma metabolomic profiling reveals metabolites robustly associated with COVID-19 severity and metabolism alterations before, during, and after disease**; Haley Chatelaine[1]; Yulu Chen[2]; John Braisted[1]; Su Chu[2]; Meryl Stav[2]; Sofina Begum[2]; Joann Diray-Arce[2]; Jaleal Sanjak[1]; Mengna Huang[2]; Jessica Lasky-Su[2]; Ewy Mathe[1]; *[1]Division of Preclinical Innovation, National Center for Advancing Translational Sciences, National Institutes of Health, Rockville, MD; [2]Channing 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 Kasahara[1]; Yasuto Yokoi[1]; Tadahiro Hoshino[1]; Akio Hayashi[2]; Hitoshi Shimano[2]; *[1]Mitsui Knowledge Industry co., ltd., Tokyo, Japan; [2]Department 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 Chiu[1]; Sin-Chen Chiang[1]; Hui-Yin Chang[2]; *[1]Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan; [2]Department 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 Yu[1]; Rohit Tripathy[1]; Brian Hoffmann[2]; Yi Li[1]; Vivek Philip[1]; *[1]The jackson laboratory, Farmington, CT; [2]The 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 Stancliffe[1]; Michaela Schwaiger-Haber[1]; Gary J. Patti[1]; *[1]Washington 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 Royer[1]; Rachel Harris[1]; Daniel Debord[1]; *[1]MOBILion Systems, Inc, Chadds Ford, PA*

ThP 335 **A deep lipidomics strategy for evaluation of cancer therapy**; Haoyue Zhang[1]; Yikun Liu[1]; Donghui Zhang[1]; Wenpeng Zhang[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China*

ThP 336 **Enzymatic Dysregulation Estimation using Lipid Network Analysis**; Tim D Rose[1, 2]; Nikolai Köhler[1]; Lisa Falk[1]; Lucie Klischat[1]; Olga E Lazareva[2, 3]; Josch K Pauling[1]; *[1]LipiTUM, Technical University of Munich, Freising, Germany; [2]EMBL, Heidelberg, Germany; [3]German Cancer Research Center (DKFZ), Heidelberg, Germany*

ThP 337 **PAMDA: Publicly Available Metabolomics Dataset Alignment and Analysis of Human Urine Measured by RPLC-MS**; Hani Habra[1]; Yamil Simon[1]; Tytus D. Mak[1]; *[1]NIST, Gaithersburg, MD*

ThP 338 **Fragmentation Site Prediction for Non-Targeted Metabolomics using Graph Neural Networks** ; Yannek Nowatzky[1]; Philipp Benner[1]; Thilo Muth[1]; *[1]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany*

ThP 339 **MS/MS-centric data processing with SIRIUS 6**; Kai Dührkop[1]; Markus Fleischauer[1]; Marcus Ludwig[1]; Martin Andre Hoffmann[1]; Fleming Kretschmer[1]; Sebastian Böcker[1]; *[1]Friedrich-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 Rudt[1]; Viola Jeck[2]; Konstantin Schwarze[2]; Ansgar Korf[2]; Matthew R. Lewis[2]; Heiko Hayen[1]; Nikolas Kessler[2]; *[1]Institute of Inorganic and Analytical Chemistry, Münster, Germany; [2]Bruker 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 Kiehne[1]; Silke Bodendiek[1]; Sofie Weinkouff[1]; Mingxun Wang[2]; Heiko Neuweger[1]; Nikolas Kessler[1]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]Department of Computer Science and Engineering, University of California Riverside, Riverside, CA*

ThP 342 **LipiDetective: a Deep Learning Framework for the Detection of Lipid Species in Mass Spectra**; Vivian J Wuerf[1]; Nikolai Köhler[1]; Florian Molnar[1]; Michael Witting[1, 2]; Josch K Pauling[1]; *[1]Technical University of Munich, Freising, Germany; [2]Helmholtz Zentrum München – German Research Center for Environmental Health, Neuherberg, Germany*

ThP 343 **The Evolving Open Access Metabolomics Resource MetaboLights**; Claire C O'Donovan[1]; Callum Martin[1]; Ozgur Yurekten[1]; Felix Amaladoss[1]; Mark Williams[1]; Thomas Payne[1]; *[1]EMBL-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. Sells[1]; Ethan Stancliffe[1]; Jacob S. Bedia[1]; Michaela Schwaiger-Haber[1]; Leah P. Shriver[1]; Gary J. Patti[1]; *[1]Washington University in St. Louis, St. Louis, MO*

ThP 345 **High-fidelity and high-performance LC-MS metabolomics data processing using asari**; Shuzhao Li[1, 2]; Amnah Siddiqa[1]; Maheshwor Thapa[1]; Shujian Zheng[1]; *[1]Jackson Laboratory, Farmington, CT; [2]University of Connecticut School of Medicine, Farmington, CT*

ThP 346 **MSPaint: A versatile Python package for visualizing mass spectrometry data**; Shaurya Chanana[1]; John T. Prince[1]; *[1]Enveda Biosciences, Boulder, CO*

ThP 347 **Combining MS2 and MS3 fragmentation spectra for the annotation of complex sphingolipids**; Brandon Y. Lieng[1]; Jeremy K. Chan[1]; Nicholas S. Ly[1]; Hannes L. Röst[1]; J. Rafael Montenegro-Burke[1]; *[1]Donnelly 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. Kozhinov[1]; Sergey Vakhrushev[2]; Yury O. Tsybin[1]; *[1]Spectroswiss, Lausanne, Switzerland; [2]University of Copenhagen, Copenhagen, Denmark*

ThP 349 **Reproducibility and challenges in analysis of large urine metabolomics datasets**; Stephen Barnes[1]; Landon S. Wilson[1]; Taylor F. Berryhill[1]; Shaoyong Su[2]; *[1]University of Alabama at Birmingham, Birmingham, AL; [2]Augusta university, Augusta, Georgia*

ThP 350 **SpectraSpectre: An implementation of MassQL for rapid querying of MS data**; Dylan J Johnson[1]; Alan K Jarmusch[2]; *[1]Integrative Bioinformatics Support Group, National Institute of Environmental Health Sciences, National Institutes of Health, Durham, North Carolina; [2]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*

ThP 351 **Library-scale assessment of spectral quality of MS/MS spectra**; Christoph A. Krettler[1]; J Taylor[1]; Tobias Kind[1]; Pelle Simpson[1]; Sarah E Haynes[1]; David Healey[1]; *[1]Enveda Biosciences, Boulder, CO*

ThP 352 **Ground-truth evaluation of high dimensional feature calling methods**; J Taylor[1]; Alex A. Kislukhin[1]; Daniel Treen[1]; Tobias Kind[1]; Sarah Haynes[1]; David Healey[1]; John T. Prince[1]; *[1]Enveda 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. Prince[1]; *[1]Enveda Biosciences, Boulder, CO*

ThP 354 **Noise Filtering in Non-targeted Metabolomics**; Iqbal Mahmud[1]; Anika Patel[1, 2]; Lin Tan[1]; Sara A Martinez[1]; Bao Tran[1]; Bo Wei[1]; Rehan Akbani[1]; Bradley Broom[1]; John Weinstein[1]; Philip L Lorenzi[1]; *[1]MD Anderson Cancer Center, Houston, TX; [2]Rice University, Houston, TX*

ThP 355 **MS/MS Spectral Alignment Enables Structural Modification Site Localization**; Mohammad Reza Zare Shahneh[1]; Mingxun Wang[2]; *[1]University of California, Riverside, Riverside, CA; [2]University 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 Iyer[2]; Caitlin E. Randolph[1]; Gaurav Chopra[1]; *[1]Purdue University Department of Chemistry, West Lafayette, IN; [2]Purdue 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. Polasky[1]; Andy T. Kong[1]; Guo Ci Teo[1]; Kevin L. Yang[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

ThP 358 **Quantification of peptidoforms in data from middle-down proteomics experiments with ProteoformQuant**; Arthur Grimaud[1]; Frederik Haugaard Holck[1]; Ole Nørregaard Jensen[1]; Veit Stefan Schwämmle[1]; *[1]University of Southern Denmark, Odense, Denmark*

ThP 359 **Estimating False Discovery Rate During Real-Time Library Search Acquisitions**; William Barshop[1]; Chris McGann[2]; Devin K Schweppe[2]; Jesse D. Canterbury[1]; *[1]Thermo Fisher Scientific, San Jose, California; [2]University of Washington, Seattle, WA*

ThP 360 **AutoMod: a new solution for uncovering protein post-translational modifications**; Hui-Yin Chang[1]; Jie-Wei Chiu[2]; Yi-Fan Chen[3]; Shuo-fu Chen[4]; Chia-Feng Tsai[5]; *[1]Department of Biomedical Sciences and Engineering, Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan; [2]Institute of Systems Biology and Bioinformatics, National Central University, Taoyuan, Taiwan; [3]Interdisciplinary Program of Engineering, National Central University, Taoyuan, Taiwan; [4]Department of Oncology, Taipei Veterans General Hospital, Taipei, Taiwan; [5]Biological 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 Ma[1]; Kellen Delaney[1]; Ashley Phetsanthad[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThP 362 **CONGA: Combining open and narrow searches with group-wise analysis**; Jack Freestone[1]; William Noble[2]; Uri Keich[1]; *[1]University of Sydney, Sydney, Australia; [2]University of Washington, Seattle, WA*

ThP 363 **An XIC-centric approach for improved identification, quantification, and reproducibility in proteomic data analyses**; Guanghui Wang[1]; Zheng Zhang[1]; Yi Liu[1]; Meghan C. Burke[1]; Sergey L. Sheetlin[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

ThP 364 **Generating spectral libraries using experimental target spectra and Prosit predicted decoy spectra**; Robert W Seymour[1]; Andy Lin[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

ThP 365 **Information content assessment of peptide fragmentation spectra using deep learning models**; Zahra Elhamraoui[1, 2]; Eva Borras[2]; Mathias Wilhelm[3]; Eduard Sabidó[1, 2]; *[1]Center for Genomic Regulation, Barcelona, Spain; [2]Universitat Pompeu Fabra Barcelona, Barcelona, Spain; [3]Technical 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 Han[1]; Eunok Paek[1]; *[1]Hanyang University, Seoul, South Korea*

ThP 367 **Prosit-PTM: One model to predict them all**; Wassim Gabriel[1]; Vitor Sternlicht[1]; Omar Shouman[1]; Rodeina Mohamed[1]; Daniel P. Zolg[2]; Ludwig Lautenbacher[1]; Bernhard Kuster[2]; Mathias Wilhelm[1]; *[1]Computational Mass Spectrometry, Technical University of Munich, Freising, Germany; [2]Chair 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 Huang[1]; Cheng-Chih Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]Department 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 Langella[5]; Mélisande Blein-Nicolas[5]; Virginie Lollier[1, 3]; Emile Benoist[4]; Géraldine Jean[4]; Guillaume Fertin[4]; Hélène Rogniaux[1, 3]; Dominique Tessier[1, 3]; *[1]INRAE, PROBE research infrastructure, BIBS facility F-44300, Nantes, France; [2]INRAE UR1268 Biopolymères Interactions Assemblage F-44316, Nantes, France; [3]INRAE UR1268 Biopolymères Interactions Assemblage F-44316 Nantes, Nantes, France; [4]LS2N, Nantes Université, Nantes Cedex 3, France; [5]Université Paris-Saclay, INRAE, CNRS,* *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 Zhang[1]; Qixin Liu[1]; Mingjie Xie[1]; Dennis Trede[2]; Tharan Srikumar[3]; Jonathan Krieger[3]; Bin Ma[1]; George Rosenberger[4]; *[1]Rapid Novor Inc., Kitchener, ON; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Bruker Ltd., Milton, ON; [4]Bruker 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 Löffler[1]; Robert L Hettich[1, 2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN*

ThP 372 **An integrative proteomics result viewer for FragPipe**; Kai Li[1]; Fengchao Yu[1]; Daniel Polasky[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

ThP 373 **Multiplexed peptide identification via iterative database search**; Chen Qian[1]; Seungjin Na[1]; Eunok Paek[1]; *[1]Hanyang 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]; *[1]VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; [2]Department 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 Hirschler[3]; Christine Carapito[3]; Sven Degroeve[1, 2]; Lennart Martens[1, 2]; Ralf Gabriels[1, 2]; *[1]VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; [2]Department of Biomolecular Medicine, Ghent University, Ghent, Belgium; [3]Laboratoire de Spectrométrie de Masse BioOrganique (LSMBO) IPHC UMR 7178, Université de Strasbourg, France*

ThP 376 **Spectroscape: validating peptide spectrum matches by real time visualization of their neighborhoods with an interactive web interface**; Long Wu[1]; Ayman Hoque[1]; Henry Lam[1]; *[1]HKUST, Hong Kong, China*

ThP 377 **De novo sequencing of ranid frogs skin peptides with the Twister algorithm**; Kira Vyatkina[1, 2, 3, 4]; Irina D. Vasileva[5]; Tatyana Y. Samgina[5]; Albert T Lebedev[5]; *[1]SPb Academic University, St Petersburg, Russia; [2]Saint Petersburg State University, St Petersburg, Russia; [3]Saint Petersburg Electrotechnical University “Leti”, St Petersburg, Russia; [4]National Research Center on Addictions, Branch of V. Serbsky NMRCPN, Moscow, Russia; [5]Lomonosov 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 Pandey[1]; Rui Zhang[2]; Qixin Liu[2]; Mingjie Xie[2]; Dennis Trede[3]; Tharan Srikumar[4]; Jonathan R Krieger[4]; Bin Ma[2]; George Rosenberger[5]; Anthony W. Purcell[6]; *[1]Monash University, Clayton, Australia; [2]Rapid Novor Inc., Kitchener, ON; [3]Bruker Dalton’s GmbH & Co KG, Bremen, Germany; [4]Bruker Ltd., Milton, ON; [5]Bruker Switzerland AG, Fällanden, Switzerland; [6]Monash University, Clayton, Australia*

ThP 379 **Algorithm Development for Analysis of Human O-GlcNAcylated Protein using LC-MS/MS**; Dasom An[1]; Jin Young Kim[2]; Heeyoun Hwang[2]; *[1]Korea Basic Science Institute, CheongJu-si, South Korea; [2]Korea Basic Science Institute, Cheoungju, South Korea*

ThP 380 **Investigating the Lipidome of ATP10d Corrected Murine Models Using LC-IM-MS with High Resolution Ion Mobility**; David C. Koomen[1]; Jody C. May[1]; Alexander J. Mansueto[1]; Todd R. Graham[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

ThP 381 **Noncovalent Copper Complexation to Differentiate Drug Enantiomers by Conventional and High Resolution Ion Mobility-Mass Spectrometry**; Benjamin K Blakley[1]; Emanuel Zlibut[1]; Allison R Reardon[1]; Jody C. May[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

ThP 382 **Characterizing the Molecular Composition of Polysorbates by High Resolution Ion Mobility-Mass Spectrometry (HRIM-HRMS)**; Kyle E Lira[1]; Allison R Reardon[1]; Jody C. May[1]; John A. McLean[1]; *[1]Vanderbilt 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 Aderorho[1]; Diana C. Velosa[2]; Shon P. Neal[2]; Christopher D. Chouinard[1]; *[1]Clemson University, Clemson, SC; [2]Florida Tech, Melbourne, FL*

ThP 384 **Brain metastasis of lung adenocarcinoma: gangliosidome investigation by ion mobility tandem mass spectrometry**; Mirela Sarbu[1]; David E. Clemmer[2]; Željka Vukelić[3]; Alina D. Zamfir[4]; *[1]National Inst for R&D in Electrochemistry and Condensed Matter, Timisoara, Romania; [2]Indiana University Bloomington, Bloomington, IN; [3]Department of Chemistry and Biochemistry, Faculty of Medicine, University of Zagreb, Zagreb, Croatia; [4]National 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 Barsch[1]; Surendar Tadi[2]; Xuejun Peng[3]; Elena Chekmeneva[4]; Katie E. Chappell[4]; Niels Goedecke[1]; Matthew R. Lewis[1]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]Bruker Daltonics, Billerica, MA; [3]Bruker Daltonics, San Jose, CA; [4]National 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 Ujma[1]; Kevin Giles[1]; Jose De Corral[2]; Keith Richardson[1]; David Langridge[1]; Dale Cooper-shepherd[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA*

ThP 387 **Coupling droplet microfluidics to cyclic ion mobility mass spectrometry for separation of isomeric small molecules**; Laura I Penabad[1]; Devin M. Makey[1]; Robert T. Kennedy[1]; Brandon T Ruotolo[1]; *[1]University 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 Butalewicz[1]; James D Sanders[1]; Nathan W. Buzitis[2]; Brian H. Clowers[2]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX; [2]Washington State University, Pullman, WA*

ThP 389 **Separation of C18:1 Fatty acid Isomers using Cyclic Ion Mobility Mass Spectrometer**; Ahsan Hameed[1, 2]; Hailemariam Abrha Assress[1, 2]; Renny S Lan[1, 2]; Mario G Ferruzzi[1, 2]; Andrew J Morris[1, 3]; *[1]Arkansas Children's Nutrition Center, Little Rock, AR; [2]University of Arkansas for Medical Sciences, Little Rock, AR; [3]Department 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 Moshkovskii[1]; Olexandr Dybkov[1]; Timo Sachsenberg[2]; Ralf Pflanz[1]; Monika Raabe[1]; Oliver Kohlbacher[2]; Henning Urlaub[1, 3]; *[1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany; [2]University of Tübingen, Tübingen, Germany; [3]University 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 Chen[1]; Josh McBee[1]; Miriam Fico[1];

Frederick G. Strathmann[1]; Daniel Debord[1]; [1]*MOBILion 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 Do[1]; Damilola S. Oluwatoba[1]; Miranda N. Limbach[1]; [1]*University of Tennessee, Knoxville, Knoxville, TN*

ThP 393 **Diagnostic Lipid Biomarkers discovery for Alzheimer's Disease using High-Resolution Ion Mobility Mass Spectrometry**; Orobola E. Olajide[1]; Kimberly Y Kartowikromo[1]; Junwei Wang[1]; Yuyan Yi[1]; Jingyi Zheng[1]; Amal K Kaddoumi[1]; Ahmed M Hamid[1]; [1]*Auburn University, AUBURN, AL*

ThP 394 **Top/Middle-Down Characterization ofα-Synuclein Glycoforms**; Kevin Jeanne Dit Fouque[1]; Samuel A. Miller[1]; Eldon Hard[2]; Matthew R. Pratt[2]; Francisco Alberto Fernandez Lima[1]; [1]*Florida International University, Miami, FL;* [2]*University 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 Kurulugama[1]; Christian Klein[1]; Harsha P. Gunawardena[2]; [1]*Agilent Technologies, Santa Clara, CA;* [2]*Janssen Research & Development, Spring House, PA*

ThP 396 **Fast Separation and Quantitation of α-, iso-α-, and β-acids via Differential Ion Mobility Spectrometry**; Emir Nazdrajić[1]; Christian Ieritano[1, 2]; Scott Hopkins[1, 2, 3]; [1]*University of Waterloo, Waterloo, ON;* [2]*Watermine Innovation, Waterloo, Ontario;* [3]*Centre 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 Lee[1]; Fanny C Liu[1]; Christian Bleiholder[1]; [1]*Florida 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 Seitz[3]; Carsten Baessmann[4]; Helen Gika[1, 2]; Georgios Theodoridis[1, 2]; [1]*Aristotle University of Thessaloniki, Thessaloniki, Greece;* [2]*Biomic AUTh, Center for Interdisciplinary Research and Innovation, Thessaloniki, Greece;* [3]*Bruker Scientific, Billerica, MA;* [4]*Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

ThP 399 **Imaging of Isomeric Metabolites in Mouse Brain with a nano-DESI timsTOF system**; Syeda Nazifa Wali[1]; Lixue Jiang[1]; Julia Laskin[1]; [1]*Purdue University, WEST LAFAYETTE, IN*

ThP 400 **In-depth identification and accurate quantification of mitochondrial and lysosomal crosstalk proteins**; Byoung-Kyu Cho[1]; Young Ah Goo[1, 2, 3]; [1]*MTAC, MGI, Washington University School of Medicine in St. Louis, St. Louis, MO;* [2]*Department of Biochemistry and Molecular Biophysics, Washington University School of Medicine in St. Louis, St. Louis, MO;* [3]*Department 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 Chatterjee[1]; Joshua A. Klein[2]; Joseph Zaia[1, 2]; [1]*Department of Biochemistry, Center for Biomedical Mass Spectrometry, Boston University Chobanian & Avedisian School of Medicine, Boston, MA;* [2]*Bioinformatics Program, Boston University, Boston, MA*

ThP 402 **Influence of MS acquisition and integration parameters on isotope ratio determinations**; Huifang Yao[1]; Haihong Zhou[1]; David McLaren[1]; Hao Chen[2]; Stephen Previs[1]; [1]*Merck & Co., Inc., Kenilworth, New Jersey;* [2]*New 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 Xu[1]; Thomas Wieloch[2]; Joshua A. M. Kaste[1]; Yair Shachar-Hill[1]; Thomas D. Sharkey[1]; [1]*Michigan State University, East Lansing, MI;* [2]*Umeå University, Umeå, Sweden*

ThP 404 **LC-MS method to determine Coenzymes (CoA) Flux**; Vasanta Putluri[1]; Abu Hena Mostafa Kamal[2]; Chandra Shekar Reddy Ambati[2]; Nagireddy Putluri[2]; [1]*Baylor College of Medicine, Houston, TX;* [2]*Baylor 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 Damont[1]; Anaïs Legrand[1]; Kathleen Rousseau[1]; Laurent Bellanger[2]; Jean-Jacques Leguay[3]; Christophe Junot[1]; François Fenaille[1]; Eric Ezan[1]; [1]*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;* [2]*Université Paris-Saclay, CEA, INRAE, Département Médicaments et Technologies pour la Santé (DMTS), SPI, Bagnols-sur-Cèze, France;* [3]*UMR 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 Harskamp[1]; Sander F. Garrelfs[2]; Jaap W. Groothoff[3]; Michiel J.S. Oosterveld[3]; Johannes B. Van Goudoever[4]; Henk Schierbeek[5]; [1]*Amsterdam UMC location University of Amsterdam, Department of Clinical Chemistry and Pediatrics, Laboratory Genetic Metabolic Diseases, Emma Children's Hospital,, Amsterdam, Netherlands;* [2]*Amsterdam UMC location University of Amsterdam, Department of Pediatric Nephrology, Emma Children's Hospital, Amsterdam, Netherlands;* [3]*Amsterdam UMC location University of Amsterdam, Department of Pediatric Nephrology, Emma Children's Hospital, Amsterdam, Netherlands;* [4]*Amsterdam UMC location University of Amsterdam, Department of Pediatrics, Emma Children's Hospital, Amsterdam, Netherlands;* [5]*Amsterdam 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 Fu[1]; Berkley J Walker[1, 2]; [1]*Department of Energy-Plant Research Laboratory, Michigan State University, East Lansing, MI;* [2]*Department 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 Tat[1]; Andrew E Paulson[1]; Young Jin Lee[1]; [1]*Iowa State University, Ames, IA*

ThP 410 **Defining nutrient inputs that fuel glioblastoma metabolism in vivo using stable-isotope tracing metabolomics**; Andrew J Scott[1]; Pietro Morlacchi[2]; Costas Lyssiotis[1]; Daniel R. Wahl[1]; [1]*University of Michigan-Ann Arbor, Ann Arbor, MI;* [2]*Agilent Technologies, Lexington, MA*

ThP 411 **A new StageTips method based on an innovative sorbent for fast and efficient peptide fractionation in proteomic studies**; Kaynoush Naraghi[1]; Mana Shafaei[2]; Michel Arotçarena[1]; Florine Hallez[1]; Cerina Chhuon[3]; Chiara Guerrera[3]; Sami Bayoudh[1]; [1]*AFFINISEP, Le Houlme, France;* [2]*Affinisep USA LLC, Miami, FL;* [3]*INSERM - US24 SFR Necker Proteome, Paris, France*

ThP 412 **Optimization of solid phase extraction pretreatment for urinary DNA adductomics by high resolution mass spectrometry**; Alexandra Keidel[1]; Carolina Möller[2]; Yuan-Jhe Chang[3]; Mu-Rong Chao[3, 4]; Jazmine Virzi[2]; Laura Deloso[2]; Theresa Evans-Nguyen[1]; Chiung-Wen Hu[5];

Marcus Cooke[2]; *[1]Department of Chemistry, University of South Florida, Tampa, Florida; [2]Oxidative Stress Group, Department of Molecular Biosciences, University of South Florida, Tampa, Florida; [3]Department of Occupational Safety and Health, Chung Shan Medical University, Taichung, Taiwan; [4]Department of Occupational Medicine, Chung Shan Medical University Hospital,, Taichung, Taiwan; [5]Department 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. Johansson[1]; Katharina Limm[1]; Katrin Hartinger[1]; Kuan-Ting Pan[1]; Nils A. Kulak[1]; *[1]PreOmics GmbH, Planegg/Martinsried, Germany*

ThP 414 **The spatial proteome study based on micro-FFPEtissues usingLCMsampling**; 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 Foster[1]; Megan Harper[1]; Nicole Kfoury[1]; Jaqueline Whitecavage[1]; *[1]Gerstel, Inc., Linthicum, MD*

ThP 416 **Mature Fully Automated Peptide Mapping**; Jason L. Richardson[1]; Zhongqi Zhang[1]; *[1]Amgen, Thousand Oaks, CA*

ThP 417 **Easy and Robust Automated Sample Preparation and Extraction for LC-MS/MS Bioanalytical Workflows**; Jonathan Danaceau[1]; Mary Trudeau[1]; Meagan Callis[1]; Steven Lai[2]; *[1]Waters Corporation, Milford, MA; [2]Waters corp, milford, MA*

ThP 418 **The effects of DDM on proteomic data in routine usage**; Xiaojing Yuan[1]; Renata Moravcova[2]; Jason C. Rogalski[1]; Leonard J. Foster[2]; *[1]Proteomics Core Facility, UBC, Vancouver, BC; [2]Department of Biochemistry and Molecular Biology, UBC, Vancouver, BC*

ThP 419 **Advanced sample preparation in LC/MS bioanalysis using new solid phase extraction**; Toshikazu Minohata[1]; Ai Tsutsui[1]; Haijuan An[2]; Keiko Shiren[1]; Satoshi Yamaki[1]; *[1]SHIMADZU Corporation, Kyoto, Japan; [2]Shimadzu (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 Oakley[5]; Jennifer J Couper[5]; Leonard C Harrison[2, 5]; John M Wentworth[2, 5]; Andrew I Webb[1, 2]; Laura F Dagley[1, 2]; *[1]Advanced Technology and Biology Division, The Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia; [2]Department of Medical Biology, University of Melbourne, Melbourne, Australia; [3]Population Health Division, The Walter and Eliza Hall Institute of Medical Research, Melbourne, Australia; [4]Faculty of Health and Medical Sciences, The University of Adelaide, Adelaide, Australia; [5]Faculty of Health and Medical Sciences, The University of Adelaide, Adelaida, 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-Jensen[1]; Florian Harking[2]; Magnus Huusfeldt[1]; Moritz Heusel[1]; Lasse Falkenby[1]; Jesper V. Olsen[2]; Nicolai Bache[1]; *[1]Evosep Biosystems, Odense, Denmark; [2]University of Copenhagen, Copenhagen, Denmark*

ThP 422 **Standardized, high-throughput platform for automated, rapid, and extensive plasma proteome characterization**; Claudia Martelli[1]; Fabian Wendt[2]; Andreas Schmidt[3]; Katrin Hartinger[4]; Gary Kruppa[5]; Nils A. Kulak[4]; Manuel Bauer[2]; *[1]Bruker Switzerland AG, Fällanden, Switzerland; [2]Tecan, Männedorf, Switzerland; [3]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [4]PreOmics GmbH, Martinsried, Germany; [5]Bruker 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 Senior[1]; Kyle Bevan[1]; Lee Williams[1]; Geoff Davies[1]; Alan Edgington[1]; Helen Lodder[1]; Russell Parry[1]; Charlotte Hayes[1]; Lucy Lund[1]; Zainab Khan[1]; Claire Desbrow[1]; Dan Menasco[1]; *[1]Biotage 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 Abreha[1]; Jasmin Johansson[2]; Zehan Hu[2]; Jonathan Krieger[3]; Katharina Limm[2]; Katrin Hartinger[2]; Nils A. Kulak[2]; *[1]PreOmics Inc., Islandia, NY; [2]PreOmics GmbH, Planegg/Martinsried, Germany; [3]Bruker 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 Hendriks[1]; Michael L Nielsen[1]; *[1]Novo 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 Kune[1]; Sylvia Tielens[2]; Maximilien Fléron[3]; Dominique Baiwir[3]; Laurent Nguyen[2]; Gauthier Eppe[1]; Gabriel Mazzucchelli[1, 3]; *[1]Laboratory of Mass Spectrometry, MolSys Research Unit, University of Liège, Liège, Belgium; [2]Laboratory of Molecular Regulation of Neurogenesis, GIGA-Stem Cells, University of Liège, Liège, Belgium; [3]GIGA Proteomics Facility, University of Liège, Liège, Belgium*

ThP 428 **Analysis of PFAS in Breast Milk: An Alternative Sample Prep**; Tina Chambers[1]; Jennifer Cottine Hitchcock[1]; *[1]Agilent 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 Apsokardu[1]; Xiaohui Zhang[1]; Guotao Lu[1]; *[1]CDS 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 Bittner[1]; Karen E. Yannell[1]; Mark Sartain[1]; Wendi A. Hale[2]; Cate Simmermaker[1]; Dustin Chang[1]; *[1]Agilent Technologies, Inc, Santa Clara, California; [2]Agilent 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 Chen[1]; Yue Song[1]; Yu-Chia Lin[2]; Shan-An Chan[3]; *[1]Agilent Technologies, Shanghai, China; [2]Great Engineer Technology Crop., Taipei, Taiwan; [3]Agilent Technologies, Taipei, Taiwan*

ThP 432 **Building a universal proteomics sample preparation platform using low-cost liquid handling robotics and 3D-printing**; Benedikt C. Clemens[1]; Eric F Zaniewski[1]; Johannas Kreuzer[1]; Soroush Hajizadeh[1]; Wilhelm Haas[1]; *[1]Massachusetts 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 Gonzalez[1]; Yanyang Hu[2]; Donna M Wang[2]; Eric T. Dziekonski[2]; R. Graham Cooks[2]; *[1]Purdue University, West Lafayette, IN; [2]Purdue University, WEST LAFAYETTE, IN*

ThP 434 **Optimization of Lipid Extraction for Untargeted Lipidomic Analysis Using Liquid Chromatography/Mass Spectrometry**; Ashraf M. Omar[1]; Qibin Zhang[1, 2]; *[1]Center for Translational Biomedical Research, University of North Carolina at Greensboro,* *North Carolina Research Campus, Kannapolis, NC; [2]Department of Chemistry & Biochemistry, University of North Carolina at Greensboro, Greensboro, NC*

ThP 435 **Elucidating the Lipidomic Dynamics of Lentiviral Production and Infection**; Joshua A Roberts[1]; Elena Godbout[2]; Christopher Boddy[3]; Jean-Simon Diallo[2]; Jeffrey C Smith[1]; *[1]Carleton University, Ottawa, ON; [2]Centre for Cancer Therapeutics, Ottawa Hospital Research Institute, Ottawa, ON; [3]University 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 Isaac[1]; Robert Plumb[1]; *[1]Waters Corporation, Milford, MA*

ThP 438 **Don't Be Ear-ritated: Kendrick Mass Defect-facilitated Determination of Triglycerides in Earwax**; Allix M. Coon[1]; Gavin Setzen[2]; Rabi A. Musah[1]; *[1]University at Albany, State University of New York, Albany, NY; [2]Albany ENT & Allergy Services, Albany, NY*

ThP 439 **Improved the detection and identification of labile lipids using Xevo™ G3 QTof Mass Spectrometer**; Nyasha C Munjoma[1]; Steven Lai[2]; Lisa Reid[1]; Jayne Kirk[1]; Lee Gethings[1]; Richard Lock[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters 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 Morstein[1]; Andrew Baker[2]; *[1]University of California San Francisco, San Francisco, CA; [2]Waters, Inc., Pleasanton, CA*

ThP 441 **How Acute Exercise Alters Rat's Lipidomic Profile of Liver**; David A Gaul[1]; Samuel G Moore[1]; Xueyun Liu[2]; Kristal Maner-Smith[2]; Eric Ortlund[2]; Karyn A Esser[3]; Laurie J Goodyear[4]; Facundo M Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Emory University, Atlanta, GA; [3]University of Florida, Gainesville, FL; [4]Harvard Medical School, Boston, MA*

ThP 442 **Variations in Lipid Profiles in the Serum Coronas Produced around Liposomal Drugs with Different Surface Properties**; Gwi Ju Jang[1]; Heeju Joung[1]; Sang Yun Han[1]; *[1]Department 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 Iglesias[1]; Gerard Hopfgartner[1]; Renzo Picenoni[2]; Guenter Boehm[2]; *[1]LSMS, Department of Inorganic and Analytical Chemistry, University of Geneva, Geneva, Switzerland; [2]CTC Analytics AG, Zwingen, Switzerland*

ThP 444 **Comprehensive lipidome profiling facilitates the discovery of targetable metabolic vulnerabilities in Group 3 medulloblastoma**; Jeremy K. Chan[1]; William D. Gwynne[1]; Andrew T. Quaile[1]; J. Rafael Montenegro-Burke[1]; *[1]Donnelly Centre for Cellular and Biomolecular Research, Toronto, ON*

ThP 445 **Untargeted lipidomics analyses of exosomes from malaria parasite-infected red cells**; Sina Feizbakhsh Bazargani[1]; Timothy Hamerly[2]; Borja Lopez-Gutierrez[2]; Rhoel R Dinglasan[2]; Timothy J. Garrett[2]; *[1]University of Florida, Gainesville, FL; [2]University 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 Marczak[1]; Katarzyna Dubkiewicz[1]; Marcin Zeman[2]; Monika Pietrowska[2]; Anna Wojakowska[1]; *[1]Institute of Bioorganic Chemistry Polish Academy of Sciences, Poznan, Poland; [2]Maria Sklodowska-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 Peterka[1]; Alessandro Maccelli[1]; Robert Jirásko[1]; Zuzana Vaňková[1]; Jakub Idkowiak[1]; Denise Wolrab[1]; Roman Hrstka[2]; Michal Holčapek[1]; *[1]University of Pardubice, Pardubice, Czech Republic; [2]Masaryk Memorial Cancer Institute, Brno, Czech Republic*

ThP 448 **The inhibition of TGFβ changed the profiles of collagen crosslinks and lipids in tumor**; Qingling Li[1]; Alessandra Castiglioni[2]; Yagai Yang[2]; Shannon Turley[2]; Rafael Cubas[2]; Wendy Sandoval[2]; *[1]Genentech, SSF; [2]Genentech Inc, South San Francisco, CA*

ThP 449 **Development of an MRM based phospholipid profiling method in human plasma using an inert C18 column**; Masaki Yamada[1]; Naoko Nagano[1]; Yutaka Umakoshi[1]; *[1]SHIMADZU Corporation, Kyoto, Japan*

ThP 450 **High-throughput UHPLC-TIMS-based lipidomics: Sub-5 min screening of plasma, cells, stool and tissues**; Eduardo Sommella[1]; Fabrizio Merciai[1]; Pietro Campiglia[1]; Erica Forsberg[2]; *[1]University of Salerno, Fisciano (SA), Italy; [2]Bruker Daltonics, San Jose, CA*

ThP 451 **Inorganic arsenic treatments alter lipidomic profiles of Escherichia coli**; Brett T Sather[1]; Hunter Fausset[1]; Scott Spurzem[1]; Garrett Gill[1]; Cole Kayser[1]; Anya Knowlton[1]; Georgia Eastham[1]; Sydney Peterson[1]; Brian Bothner[1]; *[1]Montana 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. Moustakas[3]; Eric Halls[4]; Carsten Baessmann[5]; Helen Gika[1]; *[1]Aristotle University of Thessaloniki, Thessaloniki, Greece; [2]Biomic AUTh, Center for Interdisciplinary Research and Innovation, Thessaloniki, Greece; [3]Medical School, National and Kapodistrian University of Athens, Athens, Greece; [4]Bruker Daltonics, Billerica, MA; [5]Bruker 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. Palagama[1]; Matthew J Kwiatkowski[1]; Phillip M Rzeczycki[1]; Thomas A Owen[1]; María I Morano[1]; Miguel A Gijón[1]; Paul D Kennedy[1]; Stephen D Barrett[1]; *[1]Cayman 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 Migas[4]; 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]; *[1]Vanderbilt University, Department of Biochemistry, Nashville, Tennessee; [2]Mass Spectrometry Research Center, Vanderbilt University,, Nashville, Tennessee; [3]Department of Cell and Developmental Biology, Vanderbilt University, Nashville, Tennessee; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Department of Medicine, Vanderbilt University, Nashville, Tennessee; [6]Department of Pharmacology, Vanderbilt University, Nashville, Tennessee; [7]Department 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 Meyer[1]; Yorrick R.J. Jaspers[2]; Bauke V. Schomakers[2, 3]; Jan Bert Van Klinken[2, 3, 4]; Eric Wever[2, 3]; Stephan Kemp[2]; Frédéric M. Vaz[2, 3]; Riekelt H. Houtkooper[2]; Michel Van Weeghel[2, 3]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [2]Laboratory Genetic Metabolic Diseases, Amsterdam UMC, University of Amsterdam, Amsterdam Gastroenterology Endocrinology Metabolism, Amsterdam, Netherlands; [3]Core Facility Metabolomics, Amsterdam UMC, Amsterdam, Netherlands; [4]Department of Human Genetics, Leiden University Medical Center, Leiden, Netherlands*

ThP 456 **Establishment of a global metabolomics method for Arabidopsis thaliana using high-sensitivity MS/MS on the ZenoTOF 7600 system**; Jinmei Chen[1]; Dandan Si[2]; Zhimin Long[1]; Lihai Guo[2]; *[1]SCIEX, Shanghai, China; [2]SCIEX, Beijing, China*

ThP 457 **Classification of Beef Using Metabolomics**; Zhentian Lei[1]; Saurav Sarma[2]; Carol Lorenzen[3]; Jade Cooper[4]; Lloyd Sumner[5]; *[1]University of Missouri, Columbia, MO; [2]Bayer Crop Science, St. Louis, MO; [3]Oregon State University, Corvallis, OR; [4]Texas A&M University, College Station, TX; [5]University of Missouri-Columbia, Columbia, MO*

ThP 458 **Advantages of a novel high resolution accurate mass analyzer for metabolite identification in untargeted metabolomics studies**; Siegrun Mohring[1]; Bashar Amer[2]; Susan Bird[2]; Nicolaie Eugen Damoc[1]; Martin Zeller[1]; Alexander Tiegel[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [2]Thermo Fisher Scientific, San Jose, California*

ThP 459 **A Multi-Omics Approach to Investigate Interactions between Elizabethkingia anophelis and Zika Virus**; Junyao Wang[1]; Omme Fatema Sultana[1]; Maria Onyango[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

ThP 460 **Development of Chemical Isotope Labeling LC-Orbitrap-MS for Comprehensive Analysis of small peptides**; Zhan Cheng[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*

ThP 461 **Targeted and untargeted metabolomics of mucopolysaccharidoses model in mouse liver by LC-MS/MS**; Nathan Ghafari[1]; Iskren Menkovic[2]; Pamela Lavoie[2]; Michel Boutin[2]; Christiane Auray-Blais[2]; Lekha Sleno[3]; *[1]University of Quebec in Montreal, Montreal, QC; [2]Department of Pediatrics, Division of Medical Genetics, Faculty of Medicine and Health Sciences, Sherbrooke University, Sherbrooke, QC; [3]University 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 Hayes[1]; Esther Mbuna[1]; Jaya Paudel[1]; Dr. Benjamin Bythell[1]; *[1]Ohio Universty, 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 Kang[1]; Boyeon Bae[1]; Woonhee Kim[2]; Jimin Nam[2]; Ke Li[1]; Yua Kang[1]; Chihye Chung[2]; Jeongmi Lee[1]; *[1]Sungkyunkwan University, Suwon, South Korea; [2]Konkuk University, Seoul, South Korea*

ThP 464 **Understanding the impact of sourdough starter microbiomes on bread quality**; Eva Keohane[1]; Jacqueline Chaparro[1]; Josephine Wee[2]; Charlene Van Buiten[1]; Jessica Prenni[1]; *[1]Colorado State University, Fort Collins, CO; [2]Penn State University, Centre County, Pennsylvania*

ThP 465 **Impact of Toxoplasma gondiiacute and chronic infection on organ metabolism in IL-1R−/− and WT mice**; Mahbobeh Lesani[1]; Tzu-Yu Feng[2]; Sarah E. Ewald[2]; Laura-Isobel McCall[3, 4]; *[1]university of Oklahoma, Norman, OK; [2]University of Virginia, Charlottesville, VA; [3]University of Oklahoma, Department of Microbiology and Plant Biology, Norman, OK; [4]University of Oklahoma, Department of Chemistry and Biochemistry, Norman, OK*

ThP 466 **A Novel Screening Approach for Comparing LC-MS Revered-Phase and HILIC Methods for Separations in Biological Matrices Using Amino Acid Examples**; Conner McHale[1]; Taylor Harmon[1]; *[1]Advanced Materials Technology, Wilmington, DE*

ThP 467 **Metabolic profile variation of Fragaria annanassa induce by Arthospira platensis addition, under condition of nutritional stress**; Candy Andreina Montaño-Pérez[1, 2]; Cecilia-Rocío Juárez-Rosete[1]; Juan José Ordaz-Ortíz[3]; Javier-German Rodríguez-Carpena[2]; Gabriela Ávila-Villarreal[2, 4]; *[1]Maestría Interinstitucional en Agricultura Protegida, CONACyT, Unidad Académica de Agricultura, Universidad Autónoma de Nayarit, Tepic, Mexico; [2]Unidad Especializada en I+D+i Calidad de Alimentos y Productos Naturales, Centro Nayarita de Innovación y Transferencia de Tecnología A.C., Tepic, Mexico; [3]Unidad de Genómica Avanzada, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional, CINVESTAV, (LANGEBIO), Irapuato, Mexico; [4]Unidad Académica de Ciencias Químico Biológicas y Farmacéuticas, Universidad Autónoma de Nayarit, Tepic, Mexico*

ThP 468 **Metabolomics of Colorectal Cancer for Human Serum Screening**; Kinjal Bhatt[1]; Marie-Alice Meuwis[2]; Edouard Louis[2]; Pierre-Hugues Stefanuto[1]; Jean Francois Focant[1]; *[1]University of Liege, Liege, Belgium; [2]Liege University Hospital, Liege, Belgium*

ThP 469 **System suitability testing of LC-IMS-HRMS for metabolomics applications**; Sven Wolfgang Meyer[1]; Ilmari Krebs[1]; Stefan Harsdorf[1]; Patrick Groos[1]; Jonas Wloka[1]; Erica Forsberg[1]; Matthew R. Lewis[1]; *[1]Bruker Daltonics GmbH & Co. KG, Bremen, Germany*

ThP 470 **PlantMASST: a mass spectrometry tool for mining public datasets from plants**; Paulo Wender Portal Gomes[1]; Helena Mannochio-Russo[1]; Simone Zuffa[1]; Robin Schmid[1]; Andrés Mauricio Caraballo-Rodríguez[1]; Pieter C Dorrestein[1]; *[1]Collaborative 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 Amer[1]; Christian Klaas[2]; Catharina Crone[2]; Siegrun Mohring[2]; Rahul Deshpande[1]; Claire Dauly[2]; Thomas Moehring[2]; Susan S. Bird[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

ThP 472 **Mass spectrometry analysis of the effect of hemin on Pseudomonas aeruginosa alkyl quinolone production**; Daniel J Breiner[1]; Rachel Neve[2]; Vanessa V. Phelan[3]; *[1]CU Anschutz Skaggs School of Pharmacy and Pharmaceutical Science, Aurora, CO; [2]University of Massachusetts Medical School, Worcester, MA; [3]University 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 Umakoshi[1]; Tsutomu Matsubara[2]; Chiho Kadono[2]; Yuki Sakamoto[1]; *[1]SHIMADZU Corporation, Kyoto, Japan; [2]Osaka 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 Tsai[1]; Chia-Lin Hsu[1]; Yue Song[2]; Dai-Yong Huang[3]; Shan-An Chan[4]; Yanan Yang[5]; *[1]Institute of Microbiology and Immunology, National Yang Ming Chiao Tung University, Taipei, Taiwan; [2]Agilent Technologies, Shanghai, China; [3]Agilent Technologies, Inc, Guangdong, China; [4]Agilent Technologies, Taipei, Taiwan; [5]Agilent Technologies, Santa Clara, CA*

ThP 475 **Feature-based molecular networking revealed Jasminum sambac cell extract as a powerful mixture of antioxidant metabolites**; Sara Ceccacci[1]; Adriana De Lucia[2]; Assunta Tortora[2]; Antonio Colantuono[2]; Gennaro Carotenuto[2]; Annalisa Tito[2]; Maria Chiara Monti[1]; *[1]Department of Pharmacy, University of Salerno, Fisciano, Italy; [2]Arterra Bioscience SpA, Naples, Italy*

ThP 476 **Characterization of the diurnal pattern of exhaled volatile fatty acids and enteric methane emissions of dairy cows**; Stamatios Giannoukos[1]; Zakirul Islam[2]; Susanna Räisänen[2]; Kai Wang[2]; Xiaoqi Ma[2]; Fabian Wahl[3]; Renato Zenobi[1]; Mutian Niu[2]; *[1]ETH Zurich, Zurich, Switzerland; [2]ETH Zurich, Zurich, Switzerland; [3]Agroscope, Bern, Switzerland*

ThP 477 **Investigating systemic gut microbiome derived metabolites from IL18-/- mice as potential mechanisms in health and disease**; Emily G Armitage[1]; Alan Barnes[1];

Nicholas Groth Merrild[2]; J Miotla Zarebska[2]; Neil Loftus[1]; Jonathan Swann[3]; Tonia L Vincent[2]; *[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 **ReproducibilityAnalyses ofMetabolomic Data**; Xinjian Yan[1]; Stephen E. Stein[1]; *[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. Jones[1]; Lia Ficaro[1]; Tori Rodrick[1]; Manor Askenazi[2]; Yik Siu[1]; Thomas H. Walter[3]; Kerri M. Smith[3]; Jonathan Turner[3]; Drew R. Jones[1]; *[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 Cooper[1]; Tyler K. Hunt-Smith[2]; Hunter Fausset[1]; Christa S. Merzdorf[2]; Brian Bothner[1]; *[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 Myer[1]; Eric D. Tague[1]; Christopher Bolcato[1]; Amirmansoor Hakimi[1]; Lance Shaner[2]; Laura Burns[2]; *[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 Ghosh[1]; Felice A. De Jong[2]; Chris Beecher[2]; Vladimir Shulaev[1]; *[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 Amer[1]; Siegrun Mohring[2]; Nicolaie Eugen Damoc[2]; Tabiwang N. Arrey[2]; Rahul Ravi Deshpande[1]; Daniel Hermanson[1]; Thomas Moehring[2]; Susan Bird[1]; *[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 Amer[1]; Jingjing Huang[1]; David Bergen[1]; Rahul Ravi Deshpande[1]; Vlad Zabrouskov[1]; Thomas Moehring[2]; Susan Bird[1]; *[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 Brown[1]; Shawn R. Campagna[1]; *[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 Miller[1]; Steven S Gross[1]; Marilena D'aurelio[1]; Qiuying Chen[2]; *[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. Rubio[1]; Hayley D. Ackerman[1]; John H. Lockhart[1]; Nicole R. Hackel[1]; Elsa R. Flores[1]; John M Koomen[1]; *[1]Moffitt Cancer Center, Tampa, FL*

ThP 488 **Metabolomics investigation of poly-l-lysine induced cytotoxicity**; Vahid Jahed[1, 2]; Kristine Aunina[1]; Liva Vita Kaufmane[1]; Fatemeh Rastegar Adib[1]; 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 Yedla[1]; Brandon Bills[1]; Bashar Amer[1]; Rahul Deshpande[1]; Susan Bird[1]; Vlad Zabrouskov[1]; Elys Rodriguez[2]; Uri Keshet[2]; Oliver Fiehn[2]; *[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 Stutts[1]; Yu-Chun Chiu[1]; Melissa Gronske[1]; Seth W. Kullman[1]; *[1]North Carolina State University, Raleigh, NC*

ThP 491 **Nitrilotriacetic acid-conjugated magnetic nanoparticle affinity probe-based mass spectrometry for porphyrin profiling**; Elias Gizaw Mernie[1]; Mei-Chun Tseng[2, 3]; Rofeamor P Obena[1]; Fu-Lien Huang[4]; Tzu-Ming Liu[5]; 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. Remoroza[1]; Yamil Simón-Manso[2]; Concepcion A. Remoroza[2]; William E. Wallace[2]; Stephen E. Stein[2]; Chengpeng Chen[1]; *[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 Chen[1]; Pao-Chi Liao[1]; *[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 Wangikar[1]; Damini Jaiswal[1]; Minal Nenwani[1]; *[1]Indian Institute of Technology Bombay, Mumbai, India*

ThP 495 **Metabolite structure elucidation and analysis enabled by a curated microbial biotransformation screen**; Chris J Brown[1]; Yelena Adelfinskaya[2]; Yue Fu[2, 3]; Jesse Balcer[2]; Krishna Kuppannan[2]; Yannick Djoumbou Feunang[2]; Matt Chase[2]; Elizabeth Ibwe[2]; Serge Fotso[2]; Paul Graupner[2]; David Robbins[1]; Jefferey Gilbert[2]; *[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 Abiead[1]; Wout Bittremieux[2]; Robin Schmid[3]; Simone Zuffa[1]; Justin Jj Van Der Hooft[4]; Mingxun Wang[5]; Pieter C Dorrestein[1]; *[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 Chervet[1]; Bogusław Buszewski[2]; Małgorzata Szultka-Młynska[2]; *[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 Simpson[1]; Nikolas Kessler[2]; Christopher L. Clark[3]; Heiko Neuweger[2]; *[1]Enveda Biosciences, Boulder, CO; [2]Bruker Daltonics GmbH & Co. KG, Bremen, Germany; [3]Bruker Scientific, LLC, Billerica, MA*

ThP 499 **Topic modelling improves accuracy of feature assignment in untargeted metabolomic analysis of the cancer microbiome**; Devanand M. Pinto[1]; Andrew Leslie[1]; Tracy McGaha[2]; Kenneth Chisholm[1]; *[1]NRC, Halifax, NS; [2]Princess 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 Deshpande[1]; Bashar Amer[1]; Jingjing Huang[1]; David Bergen[1]; Thomas Moehring[2]; Susan Bird[1]; *[1]Thermo Fisher Scientific, San Jose, California; [2]Thermo 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 Wallace[1]; Jess Thaxton[2, 3]; Brian P. Risenberg[2]; Katie Hurst[2]; Elizabeth Hunt[2, 4]; Brandie Ehrmann[1]; *[1]Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]Department of Department of Cell Biology & Physiology, University of North Carolina at Chapel Hill, Chapel Hill, NC; [4]2Department 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 Chen[1]; Jiangang Hu[2]; Zong Yang[3]; Bingjie Liu[3]; Lihai Guo[3]; *[1]SCIEX, Nanjing, China; [2]Shaoxing Testing Institute of Food and Drug, Shaoxing, China; [3]SCIEX, 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 Mireault[1]; Lekha Sleno[1]; *[1]University 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 Catenza[1]; Liang Li[1, 2]; *[1]University of Alberta, Edmonton, AB; [2]The Metabolomics Innovation Centre (TMIC), Edmonton, Alberta*

ThP 506 **Creation of the HoneyBee Metabolomics DataBase (HBDB)**; Armando Alcazar Magana[1]; Sofia Colmenares[1]; Jason C. Rogalski[1, 2]; Peter Awram[3]; Leonard J. Foster[4]; *[1]Life Sciences Institute, UBC, Vancouver, British Columbia; [2]UBC, Vancouver, BC; [3]Authentic Food Solutions, Vancouver, British Columbia; [4]Department 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 Luo[1]; Liang Li[2]; *[1]The Metabolomics Innovation Centre, Edmonton, AB; [2]University 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 Novak[3]; Dian Schatzmayr[3]; Isabelle P Oswald[1]; Oliver Puel[1]; Philippe Pinton[1]; *[1]Toxalim (Research Center in Food Toxicology), Toulouse university, INRAE, ENVT, INP-Purpan, Toulouse, France; [2]MetaboHUB-MetaToul, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France; [3]DSM - 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 Vilgalys[3]; Robert L. Hettich[1, 2]; Lotus Lofgren[3]; Paul E. Abraham[1, 2]; *[1]The University of Tennessee, Knoxville, Tennessee; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]Duke University, Durham, NC*

ThP 510 **Longitudinal multi-omics characterization of propyl gallate-mediated nephrotoxicity in beagles**; Nathaly Reyes Garces[1]; Weiwen Sun[1]; Si Mou[1]; Tim Hummer[2]; Xuejun Peng[3]; Alvaro Sebastian Vaca[4]; Erica Forsberg[4]; Matt Willetts[5]; Anton I. Rosenbaum[1]; Kevin Contrepois[1]; *[1]AstraZeneca, South San Francisco, CA; [2]AstraZeneca R&D, Gaithersburg, Maryland; [3]Bruker Scientific, San Jose, CA; [4]Bruker, San Jose, CA; [5]Bruker Scientific, Billerica, MA*

ThP 511 **Development of an Ion Chromatography Mass Spectrometry Platform and Spectral Library for Cancer Metabolomics**; Sara A Martinez[1]; Lin Tan[1]; Bao Tran[1]; John Weinstein[1]; Philip Lorenzi[1]; *[1]The 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 Overdahl[1]; Alan K Jarmusch[1]; *[1]National Institute of Environmental Health Sciences, Research Triangle Park, NC*

ThP 513 **A New Methodology Approach for Metabolomics Analysis of Rumen**; Kaitlyn M Melo[1]; Janet Li[1]; Sang Weon Na[2]; Mi Zhou[2]; Le Luo Guan[2]; Liang Li[1]; Shuang Zhao[1]; *[1]The Metabolomics Innovation Centre, University of Alberta, Edmonton, AB; [2]Department 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 King[1]; Christopher Jurtschenko[2]; Dale A. Cooper-Shepherd[3]; Martin Palmer[3]; Darren Hewitt[3]; Emma Marsden-Edwards[3]; *[1]Waters corporation, Wilmslow, United Kingdom; [2]Waters, Milford, MA; [3]Waters Corporation, Wilmslow, United Kingdom*

ThP 515 **Secretory response of Aspergillus niger IOC 4687 subjected to copper stress**; Silas De Almeida Perdigão Cota De Almeida[1]; Enrique Eduardo Rozas[1]; Claudio Augusto Oller Nascimento[1]; Meriellen Dias[1]; Maria Anita Mendes[1]; *[1]Dempster 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. Mofikoya[1]; Eemeli Eronen[1]; Marko Mäkinen[1]; Janne Jänis[1]; *[1]University of Eastern Finland, Department of Chemistry, Joensuu, Finland*

ThP 517 **Biochemical phenoytping of null alleles in human induced pluripotent stem cell-derived cell lineages: integrating genetics with metabolomics**; Maheshwor Thapa[1]; Shujian Zheng[1]; Nelio Oliveira[1]; Arti Taggar[1, 2]; Amnah Siddiqa[1]; Minghao Gong[1]; Anahita Amiri[1]; Justin McDonough[1]; Bill Skarnes[1, 2]; Paul Robson[1, 2]; Shuzhao Li[1, 2]; *[1]The jackson laboratory, Farmington, CT; [2]University 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 Sichilongo[1]; Tumelo Padiso[1]; Bonang B Nkoane[1]; Godiraone Tatolo[1]; Ogaufi Modisane[1]; *[1]University of Botswana, Gaborone, Botswana*

ThP 519 **Differences in metabolic profiles of patients with heart failure using high resolution GC/Q-TOF**; Sofia Nieto[1]; Luis Valdiviez[2]; Oliver Fiehn[2]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]West 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 Sartain[1]; Genevieve C. Van De Bittner[1]; Natalia Romero[2]; Yoonseok Kam[2]; Maria Apostolidi[1]; Dustin Chang[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Lexington, MA*

ThP 521 **Flexible, Vendor-agnostic Assessment of Liquid Chromatography - Mass Spectrometry System Performance using MassQL**; Heather Winter[1]; Dylan J Johnson[2]; Alan K Jarmusch[1]; *[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 Tiwari[1]; Jeramie D. Watrous[1]; Tao Long[1]; Lori Glenwinkel[1]; Igor Segota[1]; Phil Worboys[1]; Khoi Dao[1]; Edmondo Porcu[1]; Andrew Leverentz[1]; Tanya Nguyen[1]; Kim Lagerborg[1]; Vinay Bhupathy[1]; Sean Ramsey[1]; Mohit Jain[1]; *[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-Welch[4]; Bryan Wang[2, 4, 5, 6]; Peter A Kottke[1]; 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 (CMaT), 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 Zhang[1]; Jiamin Zheng[1]; Mathew Johnson[1]; Rupasri Mandal[1]; David S. Wishart[1]; *[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 Williams[1]; James L Smith[1, 2]; Thomas D Horvath[3]; Melinda A Engevik[3]; Ravi S Orugunty[2]; *[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 Evans[1]; Emily Phillips[2]; Yuqian Gao[3]; David A Gaul[2, 4]; Franklin E Leach III[5]; Brianna Garcia[6]; Kevin Cho[7]; Bradley Evans[8]; Tong Shen[9]; Shuzhao Li[10]; Timothy J. Garrett[11]; Gary J. Patti[12]; Arthur Edison[6]; Xiuxia Du[13]; Facundo Fernandez[2, 4]; Oliver Fiehn[9]; Thomas O. Metz[14]; *[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 Carolinat 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 Patil[1]; Yan Xu[2]; *[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 Dias[1]; Silas De Almeida Perdigão Cota De Almeida[1]; Enrique Eduardo Rozas Sanchez[1]; Claudio Oller Do Nascimento[1]; Ricardo Pinheiro de Souza Oliveira[2]; Maria Anita Mendes[1]; *[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 Mehta[1]; Dhavalkumar Patel[1]; Iqra Pervaiz[1]; Abraham Al-Ahmad[1]; *[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 Kim[1]; Brett Bowman[1]; Deepak Bhandari[1]; Benjamin Blount[1]; *[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. Taylor[1]; Karl F. Poncha[1]; Nicolas L. Young[1]; *[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. Rookyard[1]; Jayanta K. Chakrabarty[1]; Anu Jain[1]; Badri N. Vardarajan[2]; Min Suk Kang[2]; Lipi Das[1]; Emily G. Werth[1]; Marielba Zerlin-Esteves[3]; Lawrence S. Honig[2, 3, 4]; Lewis M. Brown[1]; 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 Gao[1]; Fanran Huang[1]; Ashok Kumar[2]; Thomas Foster[2]; Zhongwu Guo[1]; *[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 Ni[1]; Ashley Frankenfield[1]; Ling Hao[1]; *[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 Iannone[1]; Liesbeth Vereyken[1]; Farid Jahouh[1]; Elien Grajchen[1]; Sara Gorremans[1]; Luc Ver Donck[1]; Alexis Bretteville[1]; Diederik Moechars[1]; 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 Byrd[1]; Martin Wilkinson[1]; Dale A. Cooper-Shepherd[2]; Sheena E Radford[1]; Frank Sobott[1]; *[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 Zaman[1]; Yingxue Fu[1]; Ping-Chung Chen[1]; Huan Sun[1]; Shu Yang[1]; Zhiping Wu[1]; Zhen Wang[1]; Suresh Poudel[1]; Xusheng Wang[1]; Junmin Peng[1]; *[1]St jude children research hopital, Memphis, TN*

ThP 538 **Brain derived peptide abundance correlations reveal molecular subtypes of sporadic Alzheimer's disease**; Deanna Plubell[1]; Gennifer Merrihew[1]; Jea Park[1]; Chris Hsu[1]; Christine C. Wu[1]; Thomas J. Montine[2]; Michael J. MacCoss[1]; *[1]University of Washington, Seattle, WA; [2]Stanford University, Stanford, CA*

ThP 539 **Whole Blood for Analysis of Neurodegenerative Disease Biomarkers**; Wenyue Zhao[1]; Kevin P. Gillespie[1]; Teerapat Rojsajjakul[1]; Clementina Mesaros[1]; Ian Alexander Blair[1]; *[1]University 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 Brinkmalm[1]; Hlin Kvartsberg[1]; Johanna Nilsson[1]; Gunnar Brinkmalm[1]; Henrik Zetterberg[1]; Nicholas Ashton[1]; Kaj Blennow[1]; *[1]University 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 Krogsaeter[2]; Nevan J Krogan[1, 2]; Yadong Huang[1, 2]; Danielle L Swaney[1, 2]; *[1]UCSF, San Francisco, CA; [2]Gladstone Institutes, San Francisco, CA*

ThP 542 **Mass spectrometry-based metabolomics reveals methoxychlor-induced Parkinson's disease-like metabolic changes in C57BL/6 mice**; Fuyue Wang[1]; Xiaoxiao Wang[1]; Zongwei Cai[1]; *[1]State 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 Razo[1]; Michael Eyres[1]; Ping Yip[2]; Laura Ajram[1]; Andrey Gagunashvili[1]; Andrea Malaspina[2, 3]; Philippa J Hart[1]; *[1]Medicines Discovery Catapult, Manchester, United Kingdom; [2]Queen Mary University of London, East London, United Kingdom; [3]University 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 Kanshin[1]; Mitchell Martá Ariza[1]; Manon Thierry[1]; Dominique F Leitner[1]; Manor Askenazi[2]; Thomas Wisniewski[1]; Eleanor Drummond[3]; Beatrix Ueberheide[1]; *[1]NYU Grossman School of Medicine, New York, NY; [2]Biomedical Hosting LLC, Arlington, MA; [3]University 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 Shoff[1]; Hoi Ting Wu[1]; Joseph Genereux[1]; Ryan R. Julian[1]; *[1]University of California, Riverside, Riverside, CA*

ThP 546 **Large-scale, deep plasma proteomics: An 1800 sample study of Alzheimer's disease**; Asim Siddiqui[1]; Harendra Guturu[1]; Matthijs De Geus[2]; Sudeshna Das[2]; Pia Kivisakk[2]; Serafim Batzoglou[1]; Steven E Arnold[2]; *[1]Seer, Inc., Redwood City, CA; [2]Massachusetts General Hospital, Boston, MA*

ThP 547 **Proteomics method development for analysis of murine blood-brain barrier by spatially restricted in-vivo biotinylation**; Jan Schejbal[1]; Liang Jin[1]; Xue Wang[1]; Chenqi Hu[2]; Yu Tian[1]; Nadine Ruderisch[3]; *[1]AbbVie Bioresearch Center, Worcester, MA; [2]Takeda Pharmaceuticals, Cambridge, MA; [3]AbbVie, Cambridge, MA*

ThP 548 **N1-Methyladenosine in RNA Contributes to Neurodegeneration Arising from CAG Nucleotide Repeat Expansion**; Yuxiang Sun[1]; Hui Dai[2]; Xiaoxia Dai[2]; Jiekai Yin[2]; Yuxiang Cui[2]; Xiaochuan Liu[2]; Gwendolyn Gonzalez[2]; Jun Yuan[2]; Feng Tang[2]; Nan Wang[3]; Alexandra Perlegos[4]; Nancy Bonini[4]; William Yang[5]; Weifeng Gu[2]; Yinsheng Wang[2]; *[1]University of California, Riverside, RIVERSIDE, CA; [2]University of California Riverside, Riverside, CA; [3]University of California - Los Angeles, Los Angeles, CA; [4]University of Pennsylvania, Philadelphia, PA; [5]University of California, Los Angeles, Los Angeles, CA*

ThP 549 **eIF5A hypusination, boosted by dietary spermidine, protects from premature brain aging andmitochondrial dysfunction**; Yongtian Liang[1]; Chengji Piao[1]; Christine B Beuschel[1]; David Toppe[1]; Laxmikanth Kollipara[2]; Boris Bogdanow[3]; Marta Maglione[1]; Janine Lützkendorf[1]; Jason Chun Kit See[1]; Sheng Huang[1]; Tim O F Conrad[4]; Ulrich Kintscher[5]; Frank Madeo[6]; Fan Liu[3]; Albert Sickmann[7]; Stephan J Sigrist[1]; *[1]Institute for Biology/Genetics, Freie Universität Berlin, Berlin 14195, Germany; NeuroCure Cluster of Excellence, Charité Universitätmedizin Berlin, Berlin 10117, Berlin, Germany; [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Dortmund 44139, Germany, Dortmund, Germany; [3]Department of Chemical Biology, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), 13125, Berlin, Germany; [4]Institute for Mathematics and Computer Sciences, Freie Universität Berlin, Berlin 14195, Germany; Zuse Institute Berlin, Berlin 14195, Berlin, Germany; [5]German Centre for Cardiovascular Research (DZHK), partner site Berlin, Berlin 10117, Germany; Institute of Pharmacology, Center for Cardiovascular Research, Charité Universitätmedizin Berlin, Berlin 10115, Berlin, Germany; [6]Institute of Molecular Biosciences, NAWI Graz, University of Graz, Graz, Austria; BioTechMed Graz, Graz, Austria; [7]Leibniz 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. Nigro[1]; Margaret Downs[1]; Joseph Zaia[1]; Thor D. Stein[1]; Manveen K Sethi[1]; *[1]Boston 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 Xiao[1]; Yuting Xie[2]; Jinlong Gao[1]; Hui Yang[3]; Zhengyi Yang[4]; Tianzi Jiang[4]; Ying Mao[3]; Yan Li[5]; Tiannan Guo[6]; *[1]Westlake University, Hangzhou, China; [2]Westlake University, Hangzhou, China; [3]Fudan University, Shanghai, China; [4]Institute of Automation, Chinese Academy of Sciences, Beijing, China; [5]Shanghai Jiao Tong University, Shanghai, China; [6]Westlake 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 Ferron[1]; Anthony Knesis[1]; Stefan Linehan[1]; Tim Ragan[1]; Mike Sasner[2]; Katherine Stumpo[3]; Michael Easterling[3]; Mark Lim[4]; Gargey Yagnik[4]; Kenneth Rothschild[4]; *[1]TissueVision, Inc., Newton, MA; [2]The Jackson Laboratory, Bar Harbor, ME; [3]Bruker Daltonics, Billerica, MA; [4]AmberGen, Inc., Billerica, MA*

ThP 553 **CHARACTERISATION OF OLIGONUCLEOTIDES WITH PHOSPHODIESTER OR PHOSPHOROTHIOATE LINKER BY NEGATIVE ION ESI TANDEM MS AND IMS**; Fabien Hannauer[1]; John Langley[1]; Eugen Stulz[1]; Andrew D. Ray[2]; Rachelle Black[2]; Stephen W. Holman[3]; *[1]Chemistry, Faculty of Engineering and Physical Sciences, University of Southampton, Southampton, United Kingdom; [2]New Modalities Parenteral Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Macclesfield, United Kingdom; [3]Chemical 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 Doneanu[1]; Jonathan Fox[2]; Christopher Knowles[2]; Ying Qing Yu[3]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters, Milford, MA*

ThP 555 **Time-course continuous monitoring of digestion reactions increases the coverage afforded by strand-**

cleavage approaches for the characterization of larger nucleic acids; Daniele Rollo[1]; Thomas Kenderdine[1]; Ghazaleh Yassaghi[1]; Chris Bell[2]; Daniele Fabris[1, 2]; *[1]University of Connecticut, Storrs, CT; [2]RyboDynamics, Manchester, Connecticut*

ThP 556 **LC-MS/MS for Assessing DNA ADP-ribosylation**; Ting Zhao[1]; Yun Xiong[1]; *[1]University of California, Riverside, Riverside, CA*

ThP 557 **High-resolution and sensitive LC-MS/MS method for the quantification of oligonucleotides**; Dilipkumar Reddy Kandula[1]; Greg Roman[1]; Lei Xiong[2]; *[1]Sciex, Framingham, MA; [2]SCIEX, Redwood city, CA*

ThP 558 **Development of DNA CUTaMS for sensitive quantification of damage-associated DNA modifications**; Terry D Kim[1]; Ting-Yu Wang[1]; Tsui-Fen Chou[1]; Daniel R Semlow[1]; *[1]California 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 Francois[1]; Clarisse Gosset-Erard[1, 2]; Jérome Pansanel[3]; Antony Lechner[4]; Philippe Wolff[4]; Lauriane Kuhn[5]; Patrick Chaimbault[2]; *[1]Laboratoire de Spectrométrie de Masse des Interactions et des Systèmes (LSMIS) UMR 7140 (Unistra-CNRS), Université de Strasbourg, Strasbourg, France; [2]Laboratoire de Chimie et Physique-Approche Multi-échelles des Milieux Complexes (LCP-A2MC), Université de Lorraine, METZ, France; [3]Université de Strasbourg, IPHC, CNRS, UMR7178, Strasbourg, France; [4]Architecture et Réactivité de l'ARN (ARN) UPR 9002, CNRS, Université de Strasbourg, Strasbourg, France; [5]Plateforme Protéomique Strasbourg Esplanade FR 1589, CNRS, Strasbourg, France*

ThP 560 **Improved Characterization of Heavily-Modified RNA Therapeutics via Electron-Based Fragmentation Methods**; Daniel Jacob Nesbitt[1]; Trenton M. Peters-Clarke[1]; Keaton L. Mertz[1]; Michael S. Westphall[2, 3]; Trent J. Oman[4]; Joshua J. Coon[1, 2, 3, 5]; *[1]Department of Chemistry, University of Wisconsin - Madison, Madison, WI; [2]National Center for Quantitative Biology of Complex Systems, Madison, WI; [3]Department of Biomolecular Chemistry, University of Wisconsin - Madison, Madison, WI; [4]Eli Lilly and Company, Indianapolis, IN; [5]Morgridge Institute for Research, Madison, WI*

ThP 561 **Development of Micro Flow LC for RNA chemical modifications analysis using tandem mass spectrometry**; Qishan Lin[1]; Thomas Begley[1]; *[1]University at Albany, Albany, NY*

ThP 562 **Fenton reaction conditions induce 5-methylcytidine increases to E.coli transfer RNAs**; Satenik Valesyan[1]; Balasubrahmanyam Addepalli[1]; Patrick Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

ThP 563 **Stationary Phase Effects in Hydrophilic Interaction Liquid Chromatographic (HILIC) Separation of Oligonucleotides**; Scott Abernathy[1]; Patrick A. Limbach[1]; *[1]University of Cincinnati, Cincinnati, OH*

ThP 564 **Universal Mass Exclusion List for Enhanced Modification Mapping of RNA during LC-MS/MS analysis**; Asif Rayhan[1]; Balasubrahmanyam Addepalli[2]; Patrick A. Limbach[2]; *[1]Universtiy of Cincinnati, Cincinnati, OH; [2]University of Cincinnati, Cincinnati, OH*

ThP 565 **Studies on the stability and dissociation of tetramolecular RNA quadruplexes**; Anna Ploner[1]; Sarah Viola Heel[2]; Kathrin Breuker[2]; *[1]Institute of Organic Chemistry and Center for Molecular Biosciences Innsbruck (CMBI), University of Innsbruck, Innsbruck, Austria; [2]Institute 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 Bian[1]; David L Wong[2]; *[1]Agilent Technologies, Singapore, Singapore; [2]Agilent Technologies, Santa Clara, CA*

ThP 567 **Software enabled oligonucleotide mapping analysis of Erythropoietin mRNA**; Alexander Bunkowski[1]; Waltraud Evers[1]; Eckhard Belau[1]; Thomas Meid[1]; Lars Vorwerg[1]; Stuart Pengelley[1]; Yun Yang[2]; Guillaume Tremintin[2]; Detlev Suckau[1]; *[1]Bruker Daltonics, Bremen, Germany; [2]Bruker Daltonics, San Jose, CA*

ThP 568 **Optimized CID conditions for 24-75mer oligonucleotide MS/MS characterization**; Stuart Pengelley[1]; Eckhard Belau[1]; Yeni Yung-Mui[2]; Dirk Wunderlich[1]; Timo Schierling[3]; Julia Schneider[3]; Detlev Suckau[1]; *[1]Bruker Daltonics, Bremen, Germany; [2]Bruker Daltonics, San Jose, CA; [3]Axolabs GmbH, Kulmbach, Germany*

ThP 569 **Auto MSMS and targeted MSMS in-depth qualitative and quantitative analysis of oligonucleotide synthesis products and side products**; Detlev Suckau[1]; Stuart Pengelley[1]; Julia Schneider[2]; Timo Schierling[2]; Anjali Alving[3]; Eckhard Belau[1]; Konrad Winkels[1]; Lars Vorwerg[1]; Alexander Bunkowski[1]; *[1]Bruker Daltonics, Bremen, Germany; [2]Axolabs GmbH, Kulmbach, Germany; [3]Bruker Daltonics, Billerica, MA*

ThP 570 **Comprehensive Characterization of tRNA by Ultra High Performance Liquid Chromatography High Resolution Accurate Mass Spectrometry**; Robert L Ross[1]; Ryan Cowley[2]; Keeley Murphy[3]; Jennifer Sutton[4]; Min Du[3]; *[1]Thermo Fisher Scientific, Franklin, MA; [2]Thermo Fisher Scientific, Sunnyvale, CA; [3]Thermo Fisher Scientific, Cambridge, MA; [4]Thermo 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 Fukuyama[1]; Hideharu Shichi[1]; Masaki Murase[1]; Yoshihiro Yamada[1]; Sadanori Sekiya[1]; Shinichi Iwamoto[1]; Koichi Tanaka[1]; *[1]SHIMADZU Corporation, Kyoto, Japan*

ThP 572 **A simple robust method for synthetic therapeutic RNA. New chemistry, new quantitation**; Kenneth Cook[1]; Ulrik Mistarz[2]; Alexander Schwahn[3]; Keeley Murphy[4]; Yang Hao[5]; *[1]Thermofisher Scientific, Morpeth, United Kingdom; [2]Thermo Fisher Scientific, Copenhagen, Denmark; [3]Thermo Fisher Scientific, Reinach, Switzerland; [4]Thermo Fisher Scientific, Cambridge, MA; [5]Thermo Fisher Scientific, San Jose, CA*

ThP 573 **Sequence determination of long therapeutic DNA combining restriction enzyme cleavage and mass spectrometry**; Christian Sattler[1]; Aref Shahnazari[1]; Shima Marandi[1]; Andela Juric[1]; Luisa Hoffmann[1]; Burak Ceylan[1]; Michael Ruehl[1]; *[1]BioSpring Gesellschaft für Biotechnologie mbH, Frankfurt am Main, Germany*

ThP 574 **Validation of HILIC-HRMS Method for Quantitative Oligonucleotide Analysis**; Md Rabiul Islam[1]; A M Abdullah[1]; Cynthia Sommers[1]; Jason Rodriguez[1]; Deyi Zhang[2]; Darby Kozak[2]; Kui Yang[1]; *[1]Division 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; [2]Division 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 Kulkarni[1]; Robert L Ross[2]; Min Du[2]; Kate Yu[1]; *[1]908 Devices, Boston, MA; [2]Thermo 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 Li[1]; Peter Rye[2]; Vaughn Miller[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent 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 Yang[1]; Robert Ross[2];

Ryan Cowley[3]; Min Du[2]; [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 Yang[1]; Guillaume Tremintin[1]; Detlev Suckau[2]; Philip D. Compton[3]; Jared J. Drader[3]; Sheri M Wheeler[3]; [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 Tartiere[1]; Maurizio Bronzetti[1]; Stephen Kok[1]; Amy Claydon[2]; Arnd Brandenburg[3]; [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 Liu[1]; Hefeng Zhang[1]; Hongmei Wang[1]; Nan Zhao[1]; Zhiyu Li[1]; Lili Xing[1]; Yi Tao[1]; Liang Shen[1]; [1]*WuXi AppTec, Shanghai, China*

ThP 582 **Rapid Structural Analysis of Peptides by Two-Dimensional Tandem Mass Spectrometry**; My Phuong Le[1]; Dylan Holden[1]; R. Graham Cooks[1]; [1]*Purdue University, WEST LAFAYETTE, IN*

ThP 583 **Characterizing Disulfide Bonds in Cyclic Antimicrobial Peptides with Ultraviolet Photodissociation**; Jessica Hellinger[1]; Jennifer S. Brodbelt[1]; [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. Vasileva[1]; Tatyana Y. Samgina[1]; 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 Chan[1]; Henry Lam[1]; [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 Tuinstra[1]; Brian D. Thomas[1]; Steven Robinson[2]; Krzysztof Pawlak[2]; Gazmend Elezi[3]; Kym F. Faull[3]; Stephen Taylor[1]; [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 Eng[4]; Gaurav Bhardwaj[1,2,5]; Mike Guttmann[1]; [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 Roberts[1]; Ankit Jain[1]; Anne M Roberts[1]; Evan Hubbard[2]; Ryan Julian[3]; [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 Fry[1]; Evan Perez[2]; Franziska Dalhmann[2]; Ahmed Mohamed[2]; Jonathan Martens[3]; Giel Berden[3]; Theodore Corcovilos[1]; Mark A. Johnson[2]; Michael Van Stipdonk[1]; [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 Hoque[1]; Long Wu[1]; Henry Lam[1]; [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 Smyrnakis[3]; Mariangela Kosmopoulou[3]; Ajay Jha[1,2]; Kyle Fort[4]; Alexander Makarov[4]; Dimitris Papanastasiou[3]; 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. Zee[1]; Hayley Peckham[1]; Charles Farnsworth[1]; Alissa Nelson[1]; Kathryn Abell[1]; Jian Min Ren[1]; Michael Palazzola[1]; Matthew Stokes[1]; [1]*Cell Signaling Technology, Danvers, MA*

ThP 593 **Proteome-wide direct detection and quantification of protein disulfides**; Xiaolu Li[1]; Matthew Gaffrey[1]; Tong Zhang[1]; Song Feng[1]; Wei-Jun Qian[1]; [1]*Pacific Northwest National Laboratory, Richland, WA*

ThP 594 **An improved workflow for precise and comprehensive lysine acetylome analysis**; Chia-Feng Tsai[1]; Fengchao Yu[2]; Marina A Gritsenko[1]; Rosalie K. Chu[1]; Richard D. Smith[1]; Alexey Nesvizhskii[2]; Tao Liu[1]; [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 Schnatbaum[1]; Daniel P. Zolg[2]; Mathias Wilhelm[3]; Tobias Knaute[4]; Johannes Zerweck[4]; Holger Wenschuh[4]; Bernhard Kuster[2,5,6]; Ulf Reimer[4]; [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 Jacquet[1]; Gérard Hopfgartner[1]; [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. Yang[1]; Fengchao Yu[2]; Daniel A. Polasky[2]; Vadim Demichev[3]; 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 Wu[1]; Ryan R. Julian[1]; [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 Wu[1]; Dylan Tabang[2]; Hannah N. Miles[3]; Sara Sackett[4]; William A. Ricke[3,5,6]; Jon Odorico[4]; Lingjun

Li[2, 3]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Wisconsin-Madison, Department of Chemistry, Madison, WI; [3]University of Wisconsin-Madison School of Pharmacy - Madison, WI, Madison, WI; [4]University of Wisconsin-Madison, Department of Surgery, Division of Transplantation, School of Medicine and Public Health, Madison, WI; [5]University of Wisconsin-Madison, George M. O'Brien Urology Research Center of Excellence, School of Medicine and Public Health, Madison, WI; [6]University of Wisconsin-Madison, School of Medicine and Public Health,Department of Urology, Madison, WI*

ThP 601 **High-throughput Peptide Mapping for analysis of post-translational modifications and sequence variants in early development of biotherapeutics**; Vesela Encheva-Yokoya[1]; Sina Rafiee Mahmoudreza[1]; Lukas Krasny[1]; Karina Bora[1]; James Graham[1]; *[1]Lonza, London, United Kingdom*

ThP 602 **Glycosylation site mapping using highly efficient ECD in a Q-TOF**; Joseph Meeuwsen[1]; Mike Hare[1]; Rebecca Glaskin[2]; Valery Voinov[1]; Joseph Beckman[1]; *[1]e-MSion, Corvallis, OR; [2]Agilent 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]; *[1]Department of Molecular Genetics, University of Toronto, Toronto, ON; [2]Terrence Donnelly Centre for Cellular & Biomolecular Research, Toronto, Ontario; [3]Department 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 Wang[1]; Daniel M. Tremmel[3]; Sara Dutton Sackett[3]; Jon S. Odorico[3]; Lingjun Li[1, 4]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Biophysics Program, University of Wisconsin–Madison, Madison, WI; [3]Department of Surgery, Division of Transplantation, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; [4]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

ThP 605 **Arginylome Discovery Using an Unbaised Bottom-Up Proteomic Technique**; Joanna M Gongora[1]; Zongtao Lin[1]; Faith M Robison[1]; Xingyu Liu[1]; Yixuan (axe) Xie[1]; Benjamin A. Garcia[1]; *[1]Department of Biochemistry and Molecular Biophysics, Washington University in St. Louis, St Louis, MO*

ThP 606 **Identifying Isomerization of Aspartic Acid Residues in Neuropeptides**; Samuel Okyem[1]; Elena V. Romanova[2]; Jonathan V. Sweedler[3]; *[1]university of Illinois-Urbana Champaign, Urbana, IL; [2]University of Illinois Urbana Champaign, Urbana, IL; [3]University 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]; *[1]Chemical and Biological Integrative Research Center, Korea Institute of Science and Technology, Seoul, South Korea; [2]Division 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 Kasai[1]; Shiori Kuraoka[1]; Hideyuki Higashi[1]; Masanori Aikawa[1, 2, 3]; Sasha A. Singh[1]; *[1]Center for Interdisciplinary Cardiovascular Sciences, Division of Cardiovascular Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA; [2]Center for Excellence in Vascular Biology, Cardiovascular Division, Brigham and Women's Hospital, Harvard Medical School, Boston, MA; [3]Channing Division of Network Medicine, Department of Medicine, Brigham Women's Hospital, Harvard Medical School, Boston, MA*

ThP 609 **Improved performance of phosphopeptides characterization using online capillary electrophoresis coupling with ion mobility mass spectrometry (CE-IM-MS)**; Ling Ling[1]; Fuxing Xu[1]; Chuan-Fan Ding[1]; Liang Wang[2]; Kate Yu[3]; *[1]Ningbo University, Ningbo, China; [2]908 Devices, Shanghai, China; [3]908 Devices, Boston, MA*

ThP 610 **Modification Specific Modelling in PeptideProphet Improves Validation of Rare PTM Containing Peptides in Complex Samples**; David D Shteynberg[1]; Alex Zelter[2]; Nina Isoherranen[2]; Michael R Hoopmann[1]; Luis Mendoza[1]; Jimmy Eng[2]; Eric W. Deutsch[1]; Robert L. Moritz[1]; *[1]Institute for Systems Biology, Seattle, WA; [2]University 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 Riddle[3]; King CB Yabut[3]; Benjamin Zercher[4]; Alice Martynova[4]; Michael J. MacCoss[5]; Matthew F Bush[4]; Nina Isoherranen[6]; *[1]Department of Genome Sciences, University of Washington, Seattle, Washington; [2]Department of Biochemistry, University of Washington, Seattle, WA; [3]Department of Pharmaceutics, University of Washington, Seattle, Washington; [4]Department of Chemistry, University of Washington, Seattle, WA; [5]Department of Genome Sciences, University of Washington, Seattle, WA; [6]Professor 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 Juetten[1]; Jennifer Brodbelt[1]; *[1]University 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 Rocca[1]; France Baumans[1]; Christopher Kune[1]; Jean-Luc Balligand[2]; Maximilien Fléron[3]; Dominique Baiwir[3]; Gauthier Eppe[1]; Gabriel Mazzucchelli[1, 3]; *[1]Laboratory of Mass Spectrometry, MolSys Research Unit, University of Liège, Liège, Belgium; [2]Pole 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; [3]GIGA Proteomics Facility, University of Liège, Liège, Belgium*

ThP 614 **Direct determination of tyrosine sulfation sites in proteomic analysis**; Menatallah M. Youssef[1, 2]; Carson W. Szot[1]; Miriam F. Ayad[2]; Lobna A. Hussein[2]; Maha F. Abdel-Ghany[2]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Faculty of Pharmacy, Ain Shams University, Cairo, Egypt*

ThP 615 **Evaluation of MS2 Versus MS3 TMT Quantitation for Phosphotyrosine, Acetyllysine, and Methylarginine Peptides**; Alissa J. Nelson[1]; Jian Min Ren[1]; Anthony Possemato[1]; Vicky Yang[1]; Matthew Stokes[1]; *[1]CELL SIGNALING TECHNOLOGY, DANVERS, MA*

ThP 616 **Combination of the unique functions from timsTOF and ZenoTOF enables in-depth analysis of the glycoproteome**; Chi-Hung Lin[1]; Mark Marispini[1]; Wan-Fang Chou[1]; Yi (jimmy) Zeng[1]; Philip Ma[1]; Bruce Wilcox[1]; *[1]PrognomiQ Inc, San Mateo, CA*

ThP 617 **FAIMS-LC/MS Reveals Structural Heterogeneity of Isolevuglandin-adducted Peptide Autoantigens**; Daniel Roeth[1]; Nathaniel Bloodworth[2]; Wei Chen[2]; David M Patrick[2]; David G Harrison[2]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA; [2]Vanderbilt 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 Zahn[1]; Richard M Searfoss[1]; Yixuan (axe) Xie[1]; Zongtao Lin[1]; Francisca N De Luna Vitorino[1]; Benjamin A. Garcia[1]; *[1]Washington University School of Medicine, St. Louis, MO*

ThP 619 **Discovery of nitrotyrosine-containing proteins and peptides by antibody-based enrichment strategies**;

Firdous Bhat[1]; Kiran K. Mangalaparthi[1]; Joel-Sean Hsu[1]; Jane A. Peterson[2]; Husheng Ding[1]; Dong Gi Mun[1]; Akhilesh Pandey[1, 3]; *[1]Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, Minnesota; [2]Mayo Clinic, Rochester, Minnesota; [3]Center for Individualized Medicine, Mayo Clinic, Rochester, Minnesota*

ThP 620 **PASEF-DDA and one pot preparation of proteins for enrichment-free detection and quantitation of protein termini from pathogenic Mycobacteria**; Daniel D Hu[1]; Owen A Collars[1]; Patricia A Champion[1]; Matthew M Champion[1]; *[1]University of Notre Dame, Notre Dame, IN*

ThP 621 **Rapid Automated Reaction Screening and Optimization by the Unchained Labs Junior Interfaced with Open Port Interface Mass Spectrometry**; David Calabrese[1]; Nate Hoxie[1]; Pranav Bende[1]; Meghav Verma[1]; Cullen Klein[1]; John Janiszewski[1]; Alex Godfrey[1]; Sam Michael[1]; Chang Liu[2]; Thomas R. Covey[2]; *[1]NIH/NCATS, Rockville, MD; [2]SCIEX, Concord, ON*

ThP 622 **A Comparative Analysis of LC-MS Based Workflows for Host Cell Protein Analysis in Bioprocess Development**; Sachini P Karunaratne[1, 2]; Roger Liu[1]; Chris Chumsae[1]; Julia Ding[1]; *[1]Bristol Myers Squibb, Devens, MA; [2]University of Kansas, Lawrence, KS*

ThP 623 **Combining intact glycoprofiling and cell culture media analytics for in-process monitoring of an automated high-throughput multi-parallel bioreactor system**; Yun Alelyunas[1]; Charles Prochaska[2]; Clint Kukla[2]; Guillaume Bechade[3]; Patrick Boyce[3]; Mark Wrona[1]; *[1]Waters Corporation, Milford, MA; [2]Sartorius Stedim NA, Bohemia, NY; [3]Waters Corporation, Wilmslow, United Kingdom*

ThP 624 **Automating sub-unit mAb attribute screening for in-process monitoring of an automated high-throughput multi-parallel bioreactor**; Nick Pittman[1]; Patrick Boyce[1]; Caitlin Hanna[2]; Samantha Ippoliti[2]; Yun W Alelyunas[2]; Charles Prochaska[3]; Clint Kukla[3]; Guillaume Bechade[1]; Magnus Wetterhall[1]; Mark Wrona[2]; Stephan M Koza[2]; Ying Qing Yu[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]Sartorius Stedim NA, Bohemia, NY*

ThP 625 **Amino Acid Quantitation in Over 50 Mammalian Cell Culture Media with an Integrated CE-MS Analyzer**; Kenion H Blakeman[1]; Reagan Draper[1]; Zhanna Sheyner[1]; Ji Young Anderson[1]; Scott Miller[1]; *[1]908 Devices, Inc., Boston, MA*

ThP 626 **A Mass Spectrometry-Based Correlation Profiling Method for Investigating Disease Associated Alterations in Membrane Lipid-Protein Interactomes**; Liuyu Peng[1]; Richard G Lee[2]; Nichollas E Scott[1]; Aleksandra Filipovska[2]; Gavin E Reid[1]; *[1]University of Melbourne, Melbourne, Australia; [2]Telethon Kids Institute, Nedlands, Australia*

ThP 627 **Parallel evaluation of ten biotin ligases for proximity proteomics**; William Hardy[1]; Rawan Kalloush[1]; Saya Sedighi[1, 2]; Julia Kitaygorodsky[1, 2]; Vesal Kasmaeifar[1, 2]; Queenie Hu[1]; Reuben Samson[1, 2]; Brendon Seale[1]; Zhen-Yuan Lin[1]; Cassandra Wong[1]; Alexey Nesvizhskii[3, 4]; Anne-Claude Gingras[1, 2]; *[1]Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Toronto, ON; [2]Department of Molecular Genetics, University of Toronto, Toronto, ON; [3]Department of Pathology, University of Michigan, Ann Arbor, MI; [4]Department of Computational Medicine and Bioinformatics, Ann Arbor, MI*

ThP 628 **Complete structural characterization of patient-derived monoclonal autoantibodies associated with vaccine-induced thrombotic thrombocytopenia reveals the molecular mechanism of this pathology**; Daniil G Ivanov[1]; Son N Nguyen[1]; Si-Hung Le[1]; Yi Du[1]; Nikola Ivetic[2]; Ishac Nazy[2]; Igor A Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA; [2]Michael G. DeGroote School of Medicine, McMaster University, Hamilton, ON*

ThP 629 **Rapid profiling the glycosylation effects on cellular entry of SARS-CoV-2 using MALDI-MS with high mass detection**; Yuye Zhou[1, 2]; Congrui Tan[1]; Na Wu[1]; Renato Zenobi[1]; *[1]ETHZ, Zürich, Switzerland; [2]KTH Royal Institute of Techonology, Stockholm, Sweden*

ThP 630 **Native Mass Spectrometry for Determining the Effectiveness of Molecular Glues in Enhancing E3 Ligase-Protein Interactions for Targeted Protein Degradation**; Xiaojing Huang[1]; William A. Donald[1]; *[1]UNSW, Sydney, Australia*

ThP 631 **Improve sensitivity, mass resolution and accuracy in micro-SEC-MS characterization of antibody-siRNA complexes**; Jason X. Tang[1]; Zhongping Liao[1]; *[1]Eli Lilly & Company, Indianapolis, IN*

ThP 632 **Matrix-Assisted Laser Desorption/Ionization (MALDI) Studies for SARS-CoV-2 Drug Development**; Congrui Tan[1]; Yuye Zhou[1, 2]; Renato Zenobi[1]; *[1]ETH Zurich, Zurich, Switzerland; [2]KTH Royal Institute of Techonology, Stockholm, Sweden*

ThP 633 **Characterization of a Nucleotide-Binding Site at the C-Terminal Domain of Human TRAP1 by Native Mass Spectrometry and Ultraviolet Photodissociation (UVPD)**; Hanlin Ren[1]; Shanshan Yu[2]; Marcus Fischer[2]; Jennifer S. Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX; [2]St. Jude Children's Research Hospital, Memphis, TN*

ThP 634 **Quantitative Shotgun Glycomics using Concentration-Independent (COIN) Native Mass Spectrometry**; Duong T. Bui[1]; James Favell[1]; Elena N. Kitova[1]; Zhixiong Li[1]; Kelli A. McCord[1]; Edward N. Schmidt[1]; Fahima Mozaneh[1]; Matthew S. Macauley[1]; Lara K. Mahal[1]; Morris R. Flynn[1]; John S. Klassen[1]; *[1]University of Alberta, Edmonton, AB*

ThP 635 **Membrane Proteins Enrich Distinct Lipids from Natural Lipid Extracts**; Yun Zhu[1]; Melanie Odenkirk[2]; Pei Qiao[3]; Jack P. Ryan[4]; Tianqi Zhang[1]; Samantha Schrecke[1]; Ming Zhou[5]; Mike Marty[2]; Erin Baker[4]; Arthur Laganowsky[1]; *[1]Texas A&M University, College Station, TX; [2]University of Arizona, Tucson, AZ; [3]Zhejiang University of Technology, Hangzhou, China; [4]University of North Carolina at Chapel Hill, Chapel Hill, NC; [5]Baylor College of Medicine, Houston, Texas*

ThP 636 **Accurate golden standards and statistical models for co-fractionation mass spectrometry-based protein complex discovery**; Youngwoo Lee[1]; Pengcheng Yang[1]; Jun Xie[1]; Daniel Szymanski[1]; *[1]Purdue University, WEST LAFAYETTE, IN*

ThP 637 **Insights Into the Structure and Function of Polyglutamine Disease Target DNAJB6 Using Native Mass Spectrometry**; Devin M. Makey[1]; Oleta T. Johnson[2]; Laura I. Penabad[1]; Jason E. Gestwicki[2]; Robert T. Kennedy[1]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]University of California San Francisco, San Francisco, CA*

ThP 638 **Automated High-throughput Online Native MS Screening for Proteins and Protein Complexes**; Scott Kronewitter[1]; Olufemi Adeyemi[2]; Paul Gazis[3]; Ping Yip[4]; Weijing Liu[3]; Albert Konijnenberg[2]; Rosa Viner[3]; Mick Greer[5]; *[1]ThermoFisher Scientific, Cambridge, Massachusetts; [2]ThermoFisher Scientific, Eindhoven, Netherlands; [3]ThermoFisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, Boston, MA; [5]Thermo Fisher Scientific, Austin, TX*

ThP 639 **Quantifying Interactions of Methylglucose Lipopolysaccharides (MGLP) with Fatty Acids Ligands**; Elena Kitova[1]; Duong T. Bui[1]; Anna E. Grzegorzewicz[2]; Mary Jackson[2]; John S Klassen[1]; *[1]University of Alberta, Edmonton, AB; [2]Colorado State University, Fort Collins, CO*

ThP 640 **Online Coupling of Asymmetrical Flow Field-Flow Fractionation with Native Mass Spectrometry for Bio-Macromolecule Analysis**; Tao Xing[1]; Yuetian Yan[1]; Shunhai Wang[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals Inc., Tarrytown, NY*

ThP 641 **Assembly studies of a bacterial F1FO - ATP synthase using native mass spectrometry**; Alicia Just[1]; Khanh Vu Huu[1]; Nina Morgner[1]; *[1]Goethe-University, Insitute of*

Physical and Theoretical Chemistry, Frankfurt am Main, Germany

ThP 642 **Comprehensive Proteomic Interrogation of the SHOC2-MRAS-PP1C Complex**; Robert A. D'ippolito[1]; Matthew Drew[1]; Kelly Snead[1]; Dominic Esposito[1]; Frank McCormick[1, 2]; Dwight V. Nissley[1]; Caroline Dehart[1]; *[1]Frederick National Laboratory for Cancer Research, Frederick, MD; [2]Helen Diller Family Comprehensive Cancer Center, University of California, San Francisco, CA*

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]; *[1]Kavli Institute for Nanoscience Discovery, Oxford, United Kingdom; [2]Department 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]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; [3]Department of Biological Chemistry and Pharmacology, Columbus, OH*

ThP 645 **Mass spectrometric analysis of acoustically activated microdroplet mediated lipid-protein complex formation**; Cheyenne P Sircher[1]; Ashton Taylor[1]; Theresa Evans-Nguyen[1]; *[1]University of South Florida, Tampa, FL*

ThP 646 **Quantifying protein co-assembly using Native Mass Spectrometry**; Wiktoria Sadowska[1]; Justin Benesch[1]; Dominik Saman[1]; *[1]Department 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 Seale[1]; Reuben Samson[1, 2]; Isak Gerber[3]; Cassandra Wong[1]; Anne-Claude Gingras[1, 2]; *[1]Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Sinai Health, Toronto, ON; [2]University of Toronto, Toronto, ON; [3]ReSyn 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. Jayasekera[1]; Megan Ewbank[1]; Michael Thomas Marty[1]; *[1]University of Arizona, Tucson, AZ*

ThP 649 **Building a contaminant repository for proximity proteomics**; Julia Kitaygorodsky[1, 2]; Vesal Kasmaeifar[1, 2]; Geoffrey Hesketh[3]; Ugo Dionne[1]; Reuben Samson[1, 2]; William Hardy[1]; Rawan Kalloush[1]; Saya Sedighi[1, 2]; Queenie Hu[1]; Brendon Seale[1]; Zhen-Yuan Lin[1]; Cassandra Wong[1]; Alexey I. Nesvizhskii[4]; Anne-Claude Gingras[1, 2]; *[1]Lunenfeld-Tanenbaum Research Institute at Mount Sinai Hospital, Sinai Health, Toronto, ON; [2]Department of Molecular Genetics, University of Toronto, Toronto, ON; [3]Department of Biochemistry and Molecular Biology, Dalhousie University, Halifax, NS; [4]Department 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 Beer[1]; Hui Shen[2]; Michael C. Owens[2]; Qingqing Yan[1]; Phillip Wulfridge[1]; Kavitha Sarma[1]; Kathy Fange Liu[2]; Hsin-Yao Tang[1]; *[1]The Wistar Institute, Philadelphia, PA; [2]Department 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 Blue[1]; Alexis Edwards[1]; Elyssia S. Gallagher[1]; Michael A. Trakselis[1]; *[1]Baylor University, Waco, TX*

ThP 652 **Integrated Probabilistic Scoring of Protein-Protein Proximity Data Illuminates the Function of Dark Kinases**; Isaac B Plutzer[1]; Dhaval P. Bhatt[1]; Emily M. Wilkerson[1]; Dennis Goldfarb[1]; M. Ben Major[1]; *[1]Washington University School of Medicine, St. Louis, MO*

ThP 653 **Application of Crosslinking-based technology in Quantitative Analysis of PHD2 Interactome**; Haiping Ouyang[1]; Xinyu (cindy) How[1]; Xiaorong (sherry) Wang[2]; Yao Gong[1]; Lan Huang[2]; Yue Chen[1]; *[1]University of Minnesota, Minneapolis, MN; [2]University of California Irvine, Irvine, CA*

ThP 654 **Native mass spectrometry unveils the details behind the GroEL allosteric functioning mechanism**; He M Sun[1]; Thomas Walker[1]; Arthur Laganowsky[1]; Hays Rye[1]; David H. Russell[1]; *[1]Texas 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 Araoyinbo[1]; Fanny C Liu[1]; Christian Bleiholder[1]; *[1]Florida State University, Tallahassee, FL*

ThP 656 **Coupling auxin-inducible degradation with quantitative phosphoproteomics reveals a new role for PP2ARts1 in stabilizing eisosomes during mitosis.**; Andrew Demarco[1]; Mark C. Hall[2]; *[1]Purdue University, Lafayette, IN; [2]Purdue 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. Pade[1]; Jaeho Yoon[2]; Ira Daar[2]; Peter Nemes[1]; *[1]University of Maryland, College Park, College Park, MD; [2]Cancer & Developmental Biology Laboratory, National Cancer Institute, NIH, Frederick, MD*

ThP 658 **Improving Proteomics Depth with nanoLC-DIMS-TIMS-MS/MS**; Cameron D. Worthington[1]; Gary L. Glish[1]; *[1]University 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 Rivera[1]; Chunyan Li[1]; Rosalind Ang[1]; Fengqiang Wang[1]; Hongxia Wang[1]; Hillary A. Schuessler[1]; *[1]Merck & 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 Penanes[1]; Vladimir Gorshkov[1]; Mark V Ivanov[2]; Mikhail V Gorshkov[2]; Frank Kjeldsen[1]; *[1]University of Southern Denmark, Odense, Denmark; [2]Russian 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 Ser[1]; Yue Gu[2]; Jiawei Yap[2]; Yanting Lim[1]; Shi Mei Wang[1]; Nicholas RJ Gascoigne[2]; Paul A Macary[2]; Radoslaw M Sobota[1]; *[1]Institute of Molecular and Cell Biology (IMCB), Agency for Science, Technology and Research (A*STAR), Singapore, Singapore; [2]Department 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 Ma[1]; Chih-Lin Chen[1]; Cheng-Chih Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan*

ThP 663 **An in-depth plasma proteomics workflow powered by a Novel HRAM mass spectrometer**; Amirmansoor Hakimi[1]; Tabiwang N. Arrey[2]; Jeff Op De Beeck[3]; Bernard Delanghe[2]; Sally Webb[1]; Nicolaie Eugen Damoc[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; [3]Thermo Fisher Scientific - Belgium, Ghent, Belgium*

ThP 664 **A Fast and Efficient Arginine-Specific Protease for Proteomic Applications**; Chris Hosfield[1]; Jessica Wohlfahrt[2]; Jennifer Guergues[2]; Ethan Strauss[1]; Michael M. Rosenblatt[1]; Marjeta Urh[1]; Stanley Stevens Jr.[2]; *[1]Promega Corporation, Madison, WI; [2]University of South Florida, Tampa, FL*

ThP 665 **Improving Depth of Coverage and Detection of Low-Level Host Cell Proteins in Biotherapeutic Development**

with Novel Functionalized Multi-Nanoparticle Platform; Chris Sauer[1]; Elsa Gorre[1]; Xianglin Zhai[2]; Andrew Mahan[1]; Hirsh Nanda[1]; Aaron S Gajadhar[3]; Shao-yung Chen[3]; *[1]Janssen Research and Development, Spring House, PA; [2]Protein Metric Inc., Cupertino, CA; [3]Seer, Inc., Redwood City, CA*

ThP 666 **Extracellular vesicles surfaceome profiling using a DTSSP cross-linking reagent and LC-ion-mobility mass spectrometry**; Hiroyuki Katayama[1, 2]; Taketo Kato[1, 2]; Palihawadana Amungama[1]; Ranran Wu[1]; Yining Cai[1]; Fuchung Hsiao[1]; Johannes Fahrmann[1]; Jody Vykoukal[1]; Sam Hanash[1]; *[1]The University of Texas, Department of Clinical Cancer Prevention, Houston, TX; [2]Division of Thoracis Surgery, Nagoya University, Nagoya, Japan*

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Zhu, Zhijun .... WOG am 08:50
Zhu, Zhijun .... WP 462
Zhukov, Yury .... TP 196
Zhyvoloup, Alexander .... TOF pm 02:50
Zi, Jin .... MP 032
Zi, Jin .... MP 575
Zi, Jin .... TP 484
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Ziegler, Amanda .... ThP 671
Ziehm, Matthias .... TP 637
Zijlstra, Fokje .... TP 292
Žilionis, Andrius .... WP 397
Zima, Václav .... ThOE am 09:30
Zima, Václav .... TP 177
Zimmer, Jennifer .... WP 678
Zimmerman, Alan .... TP 612
Zimmerman-Federle, Hannah .... WP 011
Zimmermann, Ralf .... MOE pm 02:30
Zimmermann, Ralf .... TP 224
Zimmermann, Ralf .... WOD am 10:10
Zimmermann, Ralf .... WP 197
Zimmermann, Ralf .... WP 305
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Zimmermann, Stefan .... TP 437
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Zirem, Yanis .... WOF am 09:50
Zivkovic, Angela .... WP 050
Zivkovic, Dusan .... MOA am 10:10
Zlibut, Emanuel .... ThP 381
Zolg, Daniel .... MP 581
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Zolg, Daniel .... ThP 367
Zolg, Daniel .... ThP 595
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Zöller, Jonathan .... TOA am 08:50
Zombori, Norbert .... MP 614
Zoonens, Manuela .... TP 578
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Zou, Aimei .... ThP 053
Zou, Shaomin .... MP 161
Zou, Zhu .... MP 381
Zougman, Alexandre .... ThP 688
Zseller, Viktor .... TP 015
Zubair, Faizan .... MP 031
Zubarev, Roman .... ThP 703
Zuber, Johannes .... WP 698
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Zuliani-Alvarez, Lorena .... WP 386
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Zwiebel, Maximilian .... MP 561